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# 1 Introduction

## 1.1 Goals in this course

These are my hopes for the course. Let me know if you feel the course is not fulfilling them for you. Be free with your criticism & comments! Thanks.

- Teach basics of collective phenomena in electron systems
- Make frequent reference to real experiment and data
- Use 2nd quantized notation without field-theoretical techniques
- Get all students reading basic CM journals
- Allow students to practice presenting a talk
- Allow students to bootstrap own research if possible

## 1.2 Statistical mechanics of free Fermi gas

### 1.2.1 $T = 0$ Fermi sea

Start with simple model of electrons in metal, neglecting  $e^- - e^-$  interactions. Hamiltonian is

$$\hat{H} = - \sum_j \frac{\hbar^2 \nabla_j^2}{2m}, \quad j = 1, \dots, N \text{ particles} \quad (1)$$

Eigenstates of each  $-(\hbar^2 \nabla^2 / 2m)$  are just plane waves  $e^{i\mathbf{k} \cdot \mathbf{r}}$  labelled by  $\mathbf{k}$ , with  $k_i = 2\pi n_i / L_i$  in box with periodic B.C. Recall electrons are fermions, which means we can only put one in each single-particle state. Including spin we can put two particles ( $\uparrow\downarrow$ ) in each  $\mathbf{k}$ -state. At zero temperature the ground state of  $N$ -electron system is then formed by adding particles until we run out of electrons. Energy is  $\varepsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ , so start with two in lowest state  $k = 0$ , then add two to next states, with  $k_x$  or  $k_y$



or  $k_z = 2\pi/L$ , etc. as shown. Energy of highest particle called “Fermi energy”  $\varepsilon_F$ , magnitude of corresponding wave vector called  $k_F$ . Typical Fermi energy for metal  $\varepsilon_F \simeq 1\text{eV} \simeq 10^4 K$ . At  $T = 0$  only states with  $k < k_F$  occupied (Fermi “sea” or Fermi sphere), so we can write density of electrons as  $2^* \# \text{ occupied states/Volume}$  (2 is for spin):

$$n = \frac{2}{L^3} \sum_{k=0}^{k_F} \simeq 2 \int_{k < k_F} \frac{d^3 k}{(2\pi)^3} = \frac{1}{\pi^2} \int_0^{k_F} k^2 dk = \frac{k_F^3}{3\pi^2} \quad (2)$$

so

$$k_F = (3\pi^2 n)^{1/3} \quad \text{or} \quad \varepsilon_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m} \quad (3)$$

in other words, nothing but the density of electrons controls the Fermi energy.

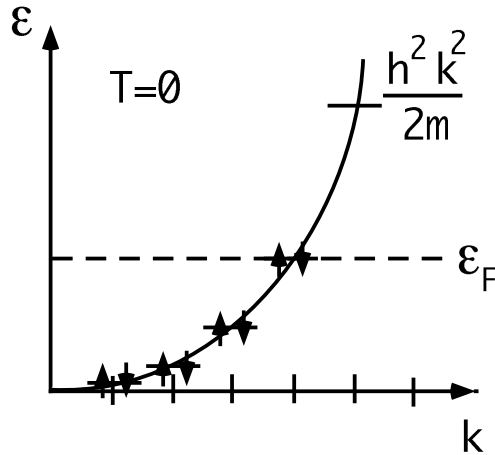


Figure 1: States of Fermi gas with parabolic spectrum,  $\varepsilon = k^2/2m$ .

The total ground state energy of the Fermi gas must be of order  $\varepsilon_F$ , since there is no other energy in the problem. If we simply add up the energies of all particles in states up to Fermi level get

$$\frac{E}{L^3} = \frac{1}{\pi^2} \int_0^{k_F} dk k^2 \left( \frac{\hbar^2 k^2}{2m} \right) = \frac{\hbar^2 k_F^5}{10\pi^2 m} \quad (4)$$

and the ground state energy per particle ( $N = nL^3$  is the total number) is

$$\boxed{\frac{E}{N} = \frac{3}{5} \varepsilon_F}. \quad (5)$$

### 1.2.2 $T > 0$ Free energy.

Reminder: partition function for free fermions in grnd conical ensemble is

$$Z = \text{Tr } e^{-\beta(\hat{H}-\mu\hat{N})} \quad (6)$$

$$= \sum_{n_1, n_2 \dots n_\infty} \langle n_1, n_2 \dots n_\infty | e^{-\beta(\hat{H}-\mu\hat{N})} | n_1, n_2 \dots n_\infty \rangle \quad (7)$$

$$= \sum_{n_1, n_2 \dots n_\infty} \langle n_1, n_2 \dots n_\infty | e^{-\beta(\sum_i [\varepsilon_i n_i - \mu n_i])} | n_1, n_2 \dots n_\infty \rangle \quad (8)$$

where  $i$  labels single-fermion state, e.g.  $i = \mathbf{k}, \sigma$ , and  $n_i$  runs from 0 to 1 for fermions. Since many-fermion state in occ. no. representation is simple product:  $|n_1, n_2 \dots n_\infty\rangle = |n_1\rangle |n_2\rangle \dots |n_\infty\rangle$ , can factorize:

$$Z = \left( \sum_{n_1} e^{-\beta[\varepsilon_1 n_1 - \mu n_1]} \right) \dots \left( \sum_{n_\infty} e^{-\beta[\varepsilon_\infty n_\infty - \mu n_\infty]} \right), \quad (9)$$

so

$$\boxed{Z = \prod_{i=0}^{\infty} (1 + e^{-\beta(\varepsilon_i - \mu)})} \quad (10)$$

Since the free energy (grand canonical potential) is  $\Omega = -k_B T \log Z$ , we get

$$\boxed{\Omega = -k_B T \sum_{i=1}^{\infty} \log (1 + e^{-\beta(\varepsilon_i - \mu)})} \quad (11)$$

### 1.2.3 Avg. fermion number.

We may want to take statistical averages of quantum operators, for which we need the *statistical operator*  $\hat{\rho} = Z^{-1} e^{-\beta(\hat{H}-\mu\hat{N})}$ . Then any operator  $\hat{\mathcal{O}}$  has an expectation value  $\langle \hat{\mathcal{O}} \rangle = \text{Tr}(\hat{\rho}\hat{\mathcal{O}})$ . For example, avg. no. of particles

$$\langle \hat{N} \rangle = \text{Tr}(\hat{\rho}\hat{N}) \quad (12)$$

$$= \frac{\text{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})} \hat{N})}{\text{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})})} \quad (13)$$

Now note this is related to derivative of  $\Omega$  wrt chem. potential  $\mu$ :

$$\frac{\partial \Omega}{\partial \mu} = -k_B T \frac{\partial \log Z}{\partial \mu} = \frac{-k_B T}{Z} \frac{\partial Z}{\partial \mu} \quad (14)$$

$$= \frac{-1}{Z} \text{Tr}(\rho \hat{N}) = -\langle \hat{N} \rangle \quad (15)$$

and using Eq. 11, we see

$$\langle \hat{N} \rangle = \sum_{i=1}^{\infty} \frac{1}{1 + e^{\beta(\varepsilon_i - \mu)}} \equiv \sum_{i=1}^{\infty} n_i^0 \quad (16)$$

where  $n_0^i$  is the avg. number of fermions in a single-particle state  $i$  in equilibrium at temperature  $T$ . If we recall  $i$  was a shorthand for  $\mathbf{k}, \sigma$ , but  $\varepsilon_{\mathbf{k}}$  doesn't depend on  $\sigma$ , we get Fermi-Dirac distribution function

$$\boxed{n_{\mathbf{k}\sigma}^0 = \frac{1}{1 + e^{\beta(\varepsilon_{\mathbf{k}} - \mu)}}} \quad (17)$$

#### 1.2.4 Fermi gas at low T.

Since the Fermi energy of metals is so high ( $\sim 10^4 K$ ), it's important to understand the limit  $k_B T \ll \varepsilon_F$ , where the Fermi gas is nearly degenerate, and make sure the classical limit  $k_B T \gg \varepsilon_F$  comes out right too. Let's calculate, for example, the entropy and specific heat, which can be obtained from the thermodynamic potential  $\Omega$  via the general thermodynamic relations

$$S = - \left( \frac{\partial \Omega}{\partial T} \right)_{V, \mu}; \quad C_V = T \left( \frac{\partial S}{\partial T} \right)_{V, \mu} \quad (18)$$

From (11) and (16), and including spin, we have

$$\begin{aligned} \Omega &= -2k_B T \sum_{\mathbf{k}} \log(1 + e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)}) \\ &= 2k_B T L^3 \int d\varepsilon N(\varepsilon) \log(1 + e^{-\beta(\varepsilon - \mu)}) \\ &\Rightarrow \\ c_V &\equiv \frac{C_V}{L^3} = 2 \frac{1}{k_B T} \int_0^{\infty} d\varepsilon N(\varepsilon) \left( \frac{-\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu)^2 \\ &= 2 \frac{1}{k_B T} \int_{-\mu}^{\infty} d\xi N(\xi) \left( \frac{-\partial f}{\partial \xi} \right) \xi^2 \end{aligned} \quad (19)$$

where I introduced the *density of  $\mathbf{k}$ -states* for one spin  $N(\varepsilon) = L^{-3} \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}})$ . The Fermi function is  $f(\varepsilon) = 1/(1 + \exp \beta(\varepsilon - \mu))$ , & I defined shifted energy variable  $\xi = \varepsilon - \mu$ . In general, the degenerate limit is characterized by  $\mathbf{k}$  sums which decay rapidly for energies far from the Fermi surface, so the game is to assume the density of states varies slowly on a scale of the thermal energy, and replace  $N(\varepsilon)$  by  $N(\varepsilon_F) \equiv N_0$ . This type of Sommerfeld expansion<sup>1</sup> assumes the density of states is a smoothly varying fctn., i.e. the thermodynamic limit  $V \rightarrow \infty$  has been taken (otherwise  $N(\varepsilon)$  is too spiky!). For a parabolic band,  $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/(2m)$  in 3D, the delta-fctn. can be evaluated to find<sup>2</sup>

$$\boxed{N(\varepsilon) = \frac{3}{2} \frac{n}{\varepsilon_F} \left( \frac{\varepsilon}{\varepsilon_F} \right)^{1/2} \theta(\varepsilon).} \quad (22)$$

This can be expanded around the Fermi level:<sup>3</sup>

$$N(\xi) = N(0) + N'(0)\xi + \frac{1}{2}N''(0)\xi^2 + \dots \quad (24)$$

(In a horrible misuse of notation,  $N(0)$ ,  $N(\varepsilon_F)$ , and  $N_0$  all mean the

---

<sup>1</sup>If you are integrating a smooth function of  $\varepsilon$  multiplied by the Fermi function derivative  $-\partial f/\partial \varepsilon$ , the derivative restricts the range of integration to a region of width  $k_B T$  around the Fermi surface. If you are integrating something times  $f(\varepsilon)$  itself, it's convenient to do an integration by parts. The result is (see e.g. Ashcroft & Mermin appendix C)

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon)|_{\varepsilon=\mu} \quad (20)$$

where  $a_n = (2 - 1/2^{2(n-1)}) \zeta(2n)$  ( $\zeta$  is Riemann  $\zeta$  fctn.,  $\zeta(2) = \pi^2/6$ ,  $\zeta(4) = \pi^4/90$ , etc.).

<sup>2</sup>Here's one way to get this:

$$N(\varepsilon) = L^{-3} \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \rightarrow \int \frac{d^3 k}{(2\pi)^3} \left| \frac{d\varepsilon}{dk} \right|^{-1} \delta(k - \frac{\sqrt{2m\varepsilon}}{\hbar}) = \int \frac{k^2 dk}{2\pi^2} \left( \frac{m}{\hbar^2 k} \right) \delta(k - \frac{\sqrt{2m\varepsilon}}{\hbar}) = \frac{3}{2} \frac{n}{\varepsilon_F} \left( \frac{\varepsilon}{\varepsilon_F} \right)^{1/2} \quad (21)$$

<sup>3</sup>When does the validity of the expansion break down? When the approximation that the density of states is a smooth function does, i.e. when the thermal energy  $k_B T$  is comparable to the splitting between states at the Fermi level,

$$\delta\varepsilon_k|_{\varepsilon_F} \simeq \frac{\hbar^2 k_F \delta k}{m} \simeq \varepsilon_F \frac{\delta k}{k_F} \simeq \varepsilon_F \frac{a}{L}, \quad (23)$$

where  $a$  is the lattice spacing and  $L$  is the box size. At  $T = 1K$ , requiring  $k_B T \sim \delta\varepsilon$ , and taking  $\varepsilon_F/k_B \simeq 10^4 K$  says that systems (boxes) of size less than  $1\mu m$  will “show mesoscopic” effects, i.e. results from Sommerfeld-type expansions are no longer valid.

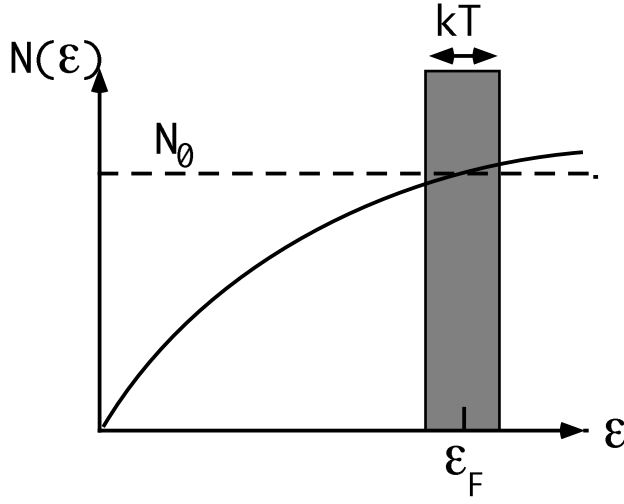


Figure 2: Density of states for parabolic spectrum,  $\varepsilon = k^2/2m$

density of states at the Fermi level). The leading order term in the low- $T$  specific heat is therefore found directly by scaling out the factors of  $T$  in Eq. (19):

$$c_V \simeq 2k_B \frac{1}{T} N_0 \int_{-\infty}^{\infty} d\xi \left( \frac{-\partial f}{\partial \xi} \right) \xi^2 = 2k_B T \underbrace{\int_{-\infty}^{\infty} dx \left( \frac{-\partial f}{\partial x} \right) x^2}_{\pi^2/3} \quad (25)$$

So

$$c_V \simeq \frac{2\pi^2}{3} N_0 k_B T + \mathcal{O}(T^3). \quad (26)$$

This is the famous linear in temperature specific heat of a free Fermi gas.<sup>4</sup>

---

<sup>4</sup>Note in (26), I extended the lower limit  $-\mu$  of the integral in Eq. (19) to  $-\infty$  since it can be shown that the chemical potential is very close to  $\varepsilon_F$  at low  $T$ . Since we are interested in temperatures  $k_B T \ll \varepsilon_F$ , and the range in the integral is only several  $k_B T$  at most, this introduces negligible error.

Why:

At  $T=0$ , the Fermi function  $n_{\mathbf{k}}^0 \rightarrow$  step function  $\theta(\mu - \varepsilon_{\mathbf{k}})$ , so we know  $\mu(T=0)$  must just be the Fermi energy  $\varepsilon_F = \hbar^2(3\pi^2 n)^{2/3}/2m$ .

$$\begin{aligned} n &= \frac{N}{L^3} = 2L^{-3} \sum_{\mathbf{k}} n_{\mathbf{k}}^0 \\ &= 2 \int d\varepsilon N(\varepsilon) f(\varepsilon) \\ &\simeq \int_{-\infty}^{\mu} d\varepsilon N(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 N'(\varepsilon)|_{\varepsilon=\mu} \quad (\text{continued on next page}) \end{aligned}$$

### 1.2.5 Classical limit.

I won't calculate the classical limit. All the standard results for a Boltzman statistics gas, e.g.  $c_V(T \gg \varepsilon_F) = (3/2)Nk_B$  follow immediately from noticing that the Fermi function reduces to the Boltzman distribution,

$$f(\varepsilon) \rightarrow e^{-\beta(\varepsilon-\mu)}, \quad T \rightarrow \infty. \quad (27)$$

(You will need to convince yourself that the classical result  $\mu/(k_B T) \rightarrow -\infty$  is recovered to make this argument.)

## 1.3 Second quantization

The idea behind the term "second quantization" arises from the fact that in the early days of quantum mechanics, forces between particles were treated classically. Momentum, position and other observables were represented by operators which do not in general commute with each other. Particle *number* is assumed to be quantized as one of the tenets of the theory, e.g. Einstein's early work on blackbody radiation.

At some point it was also realized that forces between particles are also quantized because they are *mediated* by the exchange of other particles. In Schrödinger's treatment of the H-atom the force is just the classical static Coulomb force, but a more complete treatment includes the interaction of the H-atom and its constituents with the radiation field, which must itself be quantized ("photons"). This quantization of the fields mediating the interactions between matter particles was referred to as "second" quantization. In the meantime, a second-quantized description has been developed in which *both* "matter fields" and "force fields" are described

---


$$\begin{aligned} & \simeq \underbrace{\int_{-\infty}^{\varepsilon_F} d\varepsilon N(\varepsilon)}_n + (\mu - \varepsilon_F)N(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2 N'(\varepsilon)|_{\varepsilon=\mu} \\ \Rightarrow & \boxed{\mu \simeq \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{N'(\varepsilon_F)}{N(\varepsilon_F)}} \end{aligned}$$

Since  $N'/N$  is typically of order  $1/\varepsilon_F^2$ , corrections are small.

by second-quantized field operators. In fact, modern condensed matter physics usually does go backwards and describe particles interacting via classical Coulomb forces again,<sup>5</sup> but these particles are described by field operators. Once the calculational rules are absorbed, calculating with the 2nd-quantized formalism is easier for most people than doing 1st-quantized calculations. They must, of course, yield the same answer, as they are rigorously equivalent. I will not prove this equivalence in class, as it is exceedingly tedious, but merely motivate it for you below. I urge you to read the proof once for your own edification, however.<sup>6</sup>

### 1.3.1 Symmetry of many-particle wavefunctions

Quantum mechanics allows for the possibility of indistinguishable particles, and nature seems to have taken advantage of this as a way to construct things. No electron can be distinguished from another electron, except by saying where it is, what quantum state it is in, etc. Internal quantum-mechanical consistency requires that when we write down a many-identical-particle state, we make that state noncommittal as to which particle is in which single-particle state. For example, we *say* that we have electron 1 and electron 2, and we put them in states a and b respectively, but exchange symmetry requires (since electrons are fermions) that a satisfactory wave-function has the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = A[(\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) - \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2))]. \quad (28)$$

If we have  $N$  particles, the wavefunctions must be either symmetric or antisymmetric under exchange:<sup>7</sup>

$$\Psi^B(\mathbf{r}_1 \dots \mathbf{r}_i \dots \mathbf{r}_j \dots \mathbf{r}_N) = \Psi^B(\mathbf{r}_1 \dots \mathbf{r}_j \dots \mathbf{r}_i \dots \mathbf{r}_N) \quad \text{Bosons} \quad (29)$$

$$\Psi^F(\mathbf{r}_1 \dots \mathbf{r}_i \dots \mathbf{r}_j \dots \mathbf{r}_N) = -\Psi^F(\mathbf{r}_1 \dots \mathbf{r}_j \dots \mathbf{r}_i \dots \mathbf{r}_N) \quad \text{Fermions} \quad (30)$$

---

<sup>5</sup>Q: when does this approximation break down?

<sup>6</sup>See, e.g. Fetter & Walecka, *Quantum Theory of Many-Particle Systems*

<sup>7</sup>Recently, a generalization of Bose & Fermi statistics to particles called anyons has been intensely discussed. Under exchange an anyon wavefunction behaves as  $\Psi^A(\mathbf{r}_1 \dots \mathbf{r}_i \dots \mathbf{r}_j \dots \mathbf{r}_N) = e^{i\theta} \Psi^A(\mathbf{r}_1 \dots \mathbf{r}_j \dots \mathbf{r}_i \dots \mathbf{r}_N)$  for some  $0 \leq \theta \leq 2\pi$ .

Given a set of single-particle wave functions  $\phi_{E_i}(\mathbf{r})$ , where  $E_i$  is a quantum number, e.g. energy, we can easily construct wave fctns. which satisfy statistics, e.g.

$$\Psi_{n_1 \dots n_\infty}^B(\mathbf{r}_1, \dots \mathbf{r}_N) = \left( \frac{n_1! n_2! \dots n_\infty!}{N!} \right)^{1/2} \sum_{\mathcal{P} \in \{E_1, E_2 \dots E_N\}} (\pm 1)^{\text{sgn} \mathcal{P}} \mathcal{P} \prod_{i=1}^N \phi_{E_i}(\mathbf{r}_i) \quad (31)$$

### Remarks on Eq. (31):

- sum all permutations of the  $E_i$ 's in product  $\phi_{E_1}(\mathbf{r}_1) \phi_{E_2}(\mathbf{r}_2) \dots \phi_{E_N}(\mathbf{r}_N)$ .<sup>8</sup>
- $\#$  distinct  $E_i$ 's occuring may be less than  $N$ , some missing because of multiple occupation in boson case. Example:

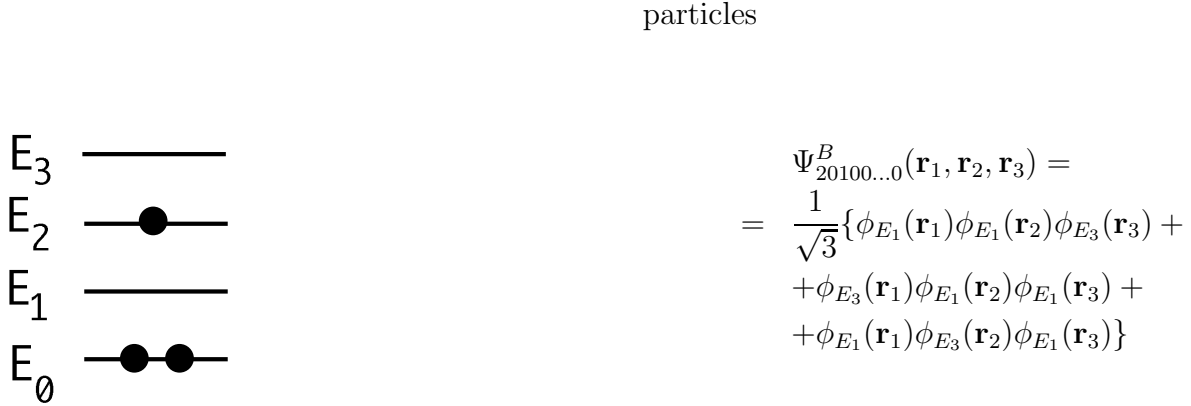


Fig. 2. Possible state of 3 noninteracting Bose

- Completely antisymmetric Fermionic wavefunction called Slater determinant:

$$\Psi_{n_1 \dots n_\infty}(\mathbf{r}_1, \dots \mathbf{r}_N) = \left( \frac{1}{N!} \right)^{1/2} \begin{vmatrix} \phi_{E_{min}}(\mathbf{r}_1) & \dots & \phi_{E_{max}}(\mathbf{r}_1) \\ \vdots & & \vdots \\ \phi_{E_{min}}(\mathbf{r}_N) & \dots & \phi_{E_{max}}(\mathbf{r}_N) \end{vmatrix} \quad (32)$$

where there are  $N$  eigenvalues which occur between  $E_{min}$  and  $E_{max}$ , inclusive, corresponding to  $N$  occupied states.

---

<sup>8</sup>You might think the physical thing to do would be to sum all permutations of the particle labels. This is correct, but actually makes things harder since one can double count if particles are degenerate (see example of 3 bosons below.) The normalization factor is chosen with the sum over all permutation of the  $E_i$ 's in mind.



### 1.3.2 Field operators

2nd quantization is alternative way of describing many body states. We describe a particle by a *field operator*

$$\hat{\psi}(\mathbf{r}) = \sum_i a_i \phi_{E_i}(\mathbf{r}) \quad (33)$$

where  $i$  runs over the quantum numbers associated with the set of eigenstates  $\phi$ ,  $a_i$  is a “coefficient” which is an operator (I’m going to neglect the hats ( $\hat{\phantom{x}}$ ) which normally denote an operator for the  $a$ ’s and  $a^\dagger$ ’s), and  $\phi_{E_i}$  is a “1st-quantized” wavefunction, i.e. a normal Schrödinger wavefunction of the type we have used up to now, such that (for example)  $H\phi_{E_i} = E_i\phi_{E_i}$ . Now we *impose* commutation relations

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')]_{\pm} = \delta(\mathbf{r} - \mathbf{r}') \quad (34)$$

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')]_{\pm} = [\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')]_{\pm} = 0, \quad (35)$$

which implies

$$[a_i, a_j^\dagger]_{\pm} = \delta_{ij} \quad ; \quad [a_i, a_j]_{\pm} = [a_i^\dagger, a_j^\dagger]_{\pm} = 0. \quad (36)$$

The upper sign is for fermions and the lower for bosons in Eqs. (35) and (36).

Now construct many-body states from vacuum (no particles)  $|0\rangle$ .  $a$  called *annihilation* operator,  $a^\dagger$  *creation operator* (see below).

Examples & comments (*all properties follow from commutation relations*):

Bosons:

- one particle in state  $i$ :  $a_i^\dagger|0\rangle \equiv |1\rangle_i$
- annihilate vacuum  $a_i|0\rangle = 0$
- (Bosons)<sup>9</sup>  $a_i^\dagger a_i^\dagger|0\rangle \equiv |2\rangle_i$

---

<sup>9</sup>Analogous state for fermions is zero, by commutation relations-check!

- (Bosons) two in  $i$  and one in  $j$ :  $a_i^\dagger a_i^\dagger a_j^\dagger |0\rangle \equiv |2\rangle_i |1\rangle_j$
- $a_i^\dagger a_i \equiv \hat{n}_i$  is *number operator* for state  $i$ .

Proof: (bosons)

$$\begin{aligned}
(a_i^\dagger a_i) |n\rangle_i &= (a_i^\dagger a_i) (a_i^\dagger)^n |0\rangle \\
&= a_i^\dagger (1 + a_i^\dagger a_i) (a_i^\dagger)^{n-1} |0\rangle = |n\rangle_i + (a_i^\dagger)^2 a_i (a_i^\dagger)^{n-1} |0\rangle \\
&= 2|n\rangle_i + (a_i^\dagger)^3 a_i (a_i^\dagger)^{n-2} |0\rangle \dots = n|n\rangle_i
\end{aligned}$$

Similarly show (bosons):<sup>10</sup>

- $a_i^\dagger |n\rangle_i = (n+1)^{1/2} |n+1\rangle_i$
- $a_i |n\rangle_i = n^{1/2} |n-1\rangle_i$
- many-particle state

$$\left( \frac{1}{n_1! n_2! \dots n_\infty!} \right)^{1/2} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \dots |0\rangle \equiv |n_1, n_2 \dots n_\infty\rangle \quad (37)$$

★ occupation numbers specify state completely, exchange symmetry included due to commutation relations! (normalization factor left for problem set)

## Fermions

- Anticommutation relations complicate matters, in particular note

$$a^2 = (a^\dagger)^2 = 0 \Rightarrow n_i = \begin{matrix} 1 \\ 0 \end{matrix} \quad (\text{Pauli principle}) \quad (38)$$

---

<sup>10</sup>By now it should be clear that the algebra for the bosonic case is identical to the algebra of simple harmonic oscillator *ladder operators*.

- SO

$$\boxed{\begin{array}{ll} a^\dagger|0\rangle = |1\rangle & a|1\rangle = |0\rangle \\ a^\dagger|1\rangle = 0 & a|0\rangle = 0 \end{array}} \quad (39)$$

- many-particle state

$$(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\dots|0\rangle \equiv |n_1, n_2 \dots n_\infty\rangle \quad (40)$$

★ note normalization factor is 1 here.

- action of creation & annihilation operators (suppose  $n_s = 1$ ):

$$\begin{aligned} a_s|\dots n_s \dots\rangle &= (-1)^{n_1+n_2+\dots n_{s-1}}(a_1^\dagger)^{n_1}\dots a_s a_s^\dagger \dots (a_\infty^\dagger)^{n_\infty}|0\rangle \\ &= (-1)^{n_1+n_2+\dots n_{s-1}}(a_1^\dagger)^{n_1}\dots (1 - \underbrace{a_s^\dagger a_s}_{=0}) \dots (a_\infty^\dagger)^{n_\infty}|0\rangle \\ &= (-1)^{n_1+n_2+\dots n_{s-1}}|\dots n_s - 1 \dots\rangle \end{aligned}$$

also

$$a_s|\dots 0 \dots\rangle = 0 \quad (41)$$

and similarly

$$a_s^\dagger|\dots n_s \dots\rangle = \begin{cases} (-1)^{n_1+n_2+\dots n_{s-1}}|\dots n_s + 1 \dots\rangle & n_s = 0 \\ 0 & n_s = 1 \end{cases} \quad (42)$$

### 1.3.3 2nd-quantized Hamiltonian

★ Point: Now “it can be shown”<sup>11</sup> that state vector

$$|\Psi(t)\rangle = \sum_{n_1, n_2 \dots n_\infty} f(n_1, n_2 \dots n_\infty, t) |n_1, n_2 \dots n_\infty\rangle \quad (43)$$

---

<sup>11</sup>Normally I hate skipping proofs. However, as mentioned above, this one is so tedious I just can't resist. The bravehearted can look, e.g. in chapter 1 of Fetter and Wallecka.

satisfies the Schrödinger equation (our old friend)

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \quad (44)$$

if we take the "2nd-quantized" form of  $\hat{H}$

$$\hat{H} = \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j + \frac{1}{2} \sum_{ijkl} a_i^\dagger a_j^\dagger \langle ij|V|kl\rangle a_l a_k \quad (45)$$

$$= \int d^3r \hat{\psi}^\dagger(\mathbf{r}) T(\mathbf{r}, \nabla_{\mathbf{r}}) \hat{\psi}(\mathbf{r}) \quad (46)$$

$$+ \frac{1}{2} \int \int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \quad (47)$$

where the 1st quantized Hamiltonian was  $H = T + V$ .

### Translationally invariant system

It may be more satisfying if we can at least verify that this formalism "works" for a special case, e.g. translationally invariant systems. For such a system the momentum  $\mathbf{k}$  is a good quantum number, so choose single-particle plane wave states

$$\phi_i(\mathbf{r}) = \phi_{\mathbf{k}\sigma}(\mathbf{r}) = L^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}} u_\sigma, \quad (48)$$

where  $u_\sigma$  is a spinor like  $u_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , etc. 1st quantized  $T$  is  $-\nabla^2/(2m)$ ,<sup>12</sup> so 2nd-quantized kinetic energy is

$$\boxed{\hat{T} \equiv \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j = \sum_{\mathbf{k}\sigma} \left( \frac{\mathbf{k}^2}{2m} \right) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}}. \quad (49)$$

Since we showed  $a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$  is just number operator which counts # of particles in state  $\mathbf{k}\sigma$ , this clearly just adds up the kinetic energy of all the occupied states, as it should. For general two-particle interaction  $V$ , let's assume  $V(\mathbf{r}, \mathbf{r}') = V(\mathbf{r} - \mathbf{r}')$  only, as must be true if we have transl. invariance. In terms of the Fourier transform

$$V(\mathbf{q}) = \frac{1}{L^3} \int d^3\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}) \quad (50)$$

---

<sup>12</sup>I'll set  $\hbar = 1$  from here on out, unless required for an honest physical calculation.

we have (steps left as exercise)

$$\hat{V} = \frac{1}{2} \sum_{\substack{\mathbf{k}, \mathbf{k}', \mathbf{q} \\ \sigma, \sigma'}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger V(\mathbf{q}) a_{\mathbf{k}'\sigma} a_{\mathbf{k}+\mathbf{q}\sigma} \quad (51)$$

### 1.3.4 Schrödinger, Heisenberg, interaction representations

Here we just give some definitions & reminders on different (equivalent) representations of quantum mechanics. In different reps., *time dependence* is associated with states (Schrödinger), operators (Heisenberg), or combination (interaction).

- **Schrödinger picture**

$$\begin{aligned} \text{state } |\hat{\psi}_S(t)\rangle, \quad \text{operators } \hat{\mathcal{O}}_S \neq \hat{\mathcal{O}}_S(t) \\ i \frac{\partial}{\partial t} |\hat{\psi}_S(t)\rangle = \hat{H} |\hat{\psi}_S(t)\rangle \end{aligned}$$

has formal solution

$$|\hat{\psi}_S(t)\rangle = e^{-i\hat{H}(t-t_0)} |\hat{\psi}_S(t_0)\rangle \quad (52)$$

Note  $\hat{H}$  hermitian  $\Rightarrow$  *time evolution operator*  $\boxed{\hat{U} \equiv e^{i\hat{H}(t-t_0)}}$  is unitary.

- **Interaction picture** (useful for pert. thy.)

$$\hat{H} = \hat{H}_0 + \hat{H}' \quad (\text{where } \hat{H}_0 \text{ usually soluble})$$

$$\begin{aligned} \text{Def. in terms of Schr. picture: } |\hat{\psi}_I(t)\rangle &= e^{i\hat{H}_0 t} |\hat{\psi}_S(t)\rangle \\ \hat{\mathcal{O}}_I(t) &= e^{i\hat{H}_0 t} \hat{\mathcal{O}}_S e^{-i\hat{H}_0 t} \end{aligned}$$

$$\Rightarrow i \frac{\partial}{\partial t} |\hat{\psi}_I(t)\rangle = \hat{H}'(t) |\hat{\psi}_I(t)\rangle$$

$$\text{with } \hat{H}'(t) = e^{i\hat{H}_0 t} \hat{H}' e^{-i\hat{H}_0 t}$$

Remarks:

- states and ops.  $t$ -dependent in interaction picture, but time dependence of operators very simple, e.g.

$$\hat{H}_0 = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$$

$$\begin{aligned} i \frac{\partial}{\partial t} a_{\mathbf{k}I}(t) &= e^{i\hat{H}_0 t} [a_{\mathbf{k}}, \hat{H}_0] e^{-i\hat{H}_0 t} \\ &= \varepsilon_{\mathbf{k}} a_{\mathbf{k}I}(t) \end{aligned}$$

$$\Rightarrow a_{\mathbf{k}I}(t) = a_{\mathbf{k}} e^{-i\varepsilon_{\mathbf{k}} t}$$

- Time evolution operator determines state at time  $t$ :

$$|\hat{\psi}_I(t)\rangle = \hat{U}(t, t_0) |\hat{\psi}_I(t_0)\rangle$$

From Schrödinger picture we find

$$\boxed{\hat{U}(t, t_0) = e^{i\hat{H}_0 t} e^{-i\hat{H}(t-t_0)} e^{-i\hat{H}_0 t_0}} \quad (53)$$

(Note  $([\hat{H}, \hat{H}_0] \neq 0!)$ )

## • Heisenberg picture

state  $|\hat{\psi}_H\rangle$   $t$ -independent,

$$\text{operators } \hat{\mathcal{O}}_H(t) = e^{i\hat{H}t} \hat{\mathcal{O}}_S e^{-i\hat{H}t}$$

so operators evolve according to *Heisenberg eqn. of motion*

$$\boxed{i \frac{\partial}{\partial t} \hat{\mathcal{O}}_H(t) = [\hat{\mathcal{O}}_H(t), H]} \quad (54)$$

★ Note—compare three reps. at  $t = 0$ :

$$|\hat{\psi}_H\rangle = |\hat{\psi}_S(0)\rangle = |\hat{\psi}_I(0)\rangle \quad (55)$$

$$\hat{\mathcal{O}}_S = \hat{\mathcal{O}}_H(0) = \hat{\mathcal{O}}_I(0) \quad (56)$$

## 1.4 Phonons

### 1.4.1 Review of simple harmonic oscillator quantization

I will simply write down some results for the standard SHO quantization from elementary QM using “ladder operators”. We consider the Hamiltonian

$$H = \frac{p^2}{2M} + \frac{K}{2}q^2 \quad (57)$$

and extract the relevant dimensions by putting

$$\begin{aligned} \omega^2 &= \frac{K}{M} \\ \xi &= q \left( \frac{M\omega}{\hbar} \right)^{1/2} \\ -i \frac{\partial}{\partial \xi} &= p (\hbar M \omega)^{-1/2} \end{aligned} \quad (58)$$

so

$$H = \frac{\hbar\omega}{2} \left( -\frac{\partial^2}{\partial \xi^2} + \xi^2 \right). \quad (59)$$

We recall soln. goes like  $e^{-\xi^2/2} H_n(\xi)$ , where  $H_n$  are Hermite polynomials, and that eigenvalues are

$$E_n = \hbar\omega(n + 1/2) \quad (60)$$

Define *ladder operators*  $a, a^\dagger$  as

$$a = \frac{1}{\sqrt{2}} \left( \xi + \frac{\partial}{\partial \xi} \right) \quad (61)$$

$$a^\dagger = \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \quad (62)$$

Ladder ops. obey commutation relations (check)

$$[a, a^\dagger] = 1 \quad ; \quad [a, a] = 0 \quad ; \quad [a^\dagger, a^\dagger] = 0 \quad (63)$$

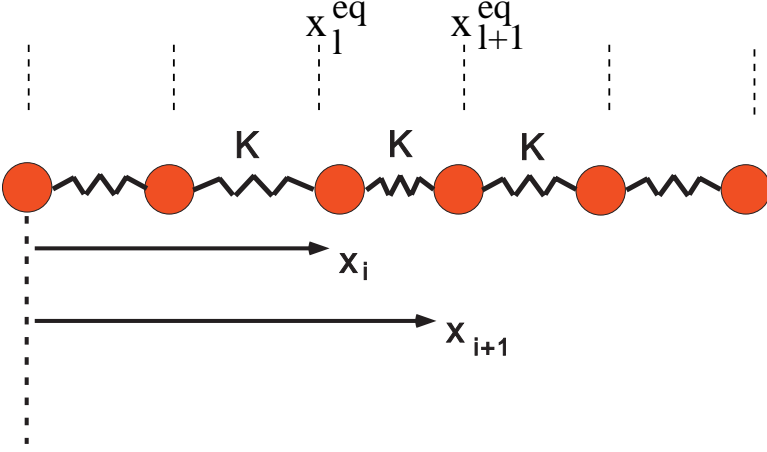


Figure 3: Linear chain with spring couplings  $K$ . Dynamical variables are  $q_i \equiv x_i - x_i^{eq}$

& then  $H$  may be written (check)

$$H = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right). \quad (64)$$

$a, a^\dagger$  connect eigenstates of different quantum nos.  $n$ , as

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}} |0\rangle, \quad (65)$$

where  $|0\rangle$  is state which obeys  $a|0\rangle = 0$ . Operating on  $|n\rangle$  with  $a^\dagger$  may be shown with use of commutation relations to give

$$a^\dagger |n\rangle = (n + 1/2)^{1/2} |n + 1\rangle \quad ; \quad a |n\rangle = n^{1/2} |n - 1\rangle \quad (66)$$

so with these defs. the ladder operators for SHO are seen to be *identical* to *boson* creation and annihilation operators defined above in Sec. 1.3.2.

### 1.4.2 1D harmonic chain

If we now consider  $N$  atoms on a linear chain, each attached to its neighbor with a “spring” of spring constant  $K$  as shown in figure. First let’s consider the problem classically. The Hamiltonian is

$$H = \sum_{\ell} \frac{p_{\ell}^2}{2m} + \frac{K}{2} (q_{\ell} - q_{\ell+1})^2, \quad (67)$$



where the  $q_\ell$ 's are the displacements from atomic equilibrium positions. Now Hamilton's eqns. (or Newton's 2nd law!) yield

$$-M\ddot{q}_j = M\omega^2 q_j = K(2q_j - q_{j-1} - q_{j+1}). \quad (68)$$

A standing sinusoidal wave  $q_j = A \cos(ka_j)$  satisfies this equation *if* the eigenfrequencies have the form

$$\omega_k^2 = \frac{K}{M} 2(1 - \cos ka), \quad (69)$$

where if  $a$  is the lattice constant,  $k = 2\pi/\lambda$ . Note that for small  $k$ ,  $\omega_k$  is linear,  $\omega_k \simeq (K/M)^{1/2} ka$ .<sup>13</sup>

This is the *classical* calculation of the normal modes of oscillation on a 1D chain. To quantize the theory, let's *impose* canonical commutation relations on the position and momentum of the  $\ell$ th and  $j$ th atoms:

$$[q_\ell, p_j] = i\hbar \delta_{\ell m} \quad (70)$$

and construct collective variables which describe the modes themselves (recall  $k$  is wave vector,  $\ell$  is position) :

$$\begin{aligned} q_\ell &= \frac{1}{N^{1/2}} \sum_k e^{ikal} Q_k \quad ; \quad Q_k = \frac{1}{N^{1/2}} \sum_\ell e^{-ikal} q_\ell \\ p_\ell &= \frac{1}{N^{1/2}} \sum_k e^{-ikal} p_k \quad ; \quad P_k = \frac{1}{N^{1/2}} \sum_\ell e^{ikal} p_\ell, \end{aligned} \quad (71)$$

which leads to canonical commutation relations in wave vector space:

$$\begin{aligned} [Q_k, P_{k'}] &= \frac{1}{N} \sum_{\ell, m} e^{-ikal} e^{ik'am} [q_\ell, p_m] \\ &= \frac{i\hbar}{N} \sum_\ell e^{-ial(k-k')} = i\hbar \delta_{k, k'}. \end{aligned} \quad (72)$$

Let's now express the Hamiltonian (67) in terms of the new variables. We have, with a little algebra and Eq. (69),

$$\begin{aligned} \sum_\ell p_\ell^2 &= \sum_k P_k P_{-k} \\ \frac{K}{2} \sum_\ell (q_\ell - q_{\ell-1})^2 &= \frac{K}{2} \sum_k Q_k Q_{-k} (2 - e^{ika} - e^{-ika}) = \frac{M}{2} \sum_k \omega_k^2 Q_k Q_{-k} \end{aligned} \quad (73)$$

---

<sup>13</sup>Note since  $k = 2\pi n/(Na)$ , the  $\omega_k$  are *independent of system size*

so

$$\boxed{H = \frac{1}{2M} \sum_k p_k p_{-k} + \frac{M}{2} \sum_k \omega_k^2 Q_k Q_{-k}}. \quad (74)$$

Note that the energy is now expressed as the sum of kinetic + potential energy of each *mode*  $k$ , and there is no more explicit reference to the motion of the atomic constituents. To *second quantize* the system, we write down creation and annihilation operators for each mode  $k$ . Define

$$a_k = \left( \frac{M\omega_k}{2\hbar} \right)^{1/2} \left( Q_k + \frac{i}{M\omega_k} P_{-k} \right) \quad (75)$$

$$a_k^\dagger = \left( \frac{M\omega_k}{2\hbar} \right)^{1/2} \left( Q_{-k} - \frac{i}{M\omega_k} P_k \right) \quad (76)$$

which can be shown, just as in the single SHO case, to obey commutation relations

$$[a_k, a_{k'}^\dagger] = \delta_{kk'} \quad (77)$$

$$[a_k, a_{k'}] = 0 \quad (78)$$

$$[a_k^\dagger, a_{k'}^\dagger] = 0 \quad (79)$$

and the Hamiltonian expressed simply as

$$\sum_k \hbar\omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) \quad (80)$$

which we could have probably guessed if we had realized that since the normal modes don't interact, we have simply the energy of all allowed harmonic oscillators. Note this is a *quantum* Hamiltonian, but the energy scale in  $H$  is the *classical* mode frequency  $\omega_k$ .

### 1.4.3 Debye Model

Let us imagine using the Hamiltonian (80) as a starting point to calculate the specific heat of a (3D) solid due to phonons. We take the Debye model for the dispersion to simplify the calculation,

$$\omega_{\mathbf{k}} = \begin{cases} ck & k < k_D \\ 0 & k > k_D \end{cases} \quad (81)$$

where the Debye wave vector  $k_D = (6\pi^2 n)^{1/3}$  is obtained by replacing the first Brillouin zone of the solid by a sphere of radius  $k_D$  which contains  $N$  wave vectors, with  $N$  the number of ions in the crystal. The average value of the Hamiltonian is

$$U = \langle H \rangle = 3 \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left( \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle + \frac{1}{2} \right) = 3 \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left( \frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}} - 1} + \frac{1}{2} \right) \quad (82)$$

since the average number of phonons in state  $\mathbf{k}$  is simply the expectation value of a boson number operator

$$\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \equiv \text{Tr}(\rho a_{\mathbf{k}}^\dagger a_{\mathbf{k}}) = b(\hbar \omega_{\mathbf{k}}), \quad (83)$$

where  $b(x) = (\exp(\beta x) - 1)^{-1}$  is the free Bose distribution function. The factors of 3 come from the 3 independent phonon polarizations, which we consider to be degenerate here. Taking one derivative wrt temperature, the spec. heat per unit volume is

$$\begin{aligned} c_V &= \left. \frac{\partial u}{\partial T} \right|_n = 3 \frac{\partial}{\partial T} \sum_{\mathbf{k}} \frac{\hbar c k}{e^{\beta \hbar c k} - 1} = 3 \frac{\partial}{\partial T} \frac{\hbar c}{2\pi^2} \int_0^{k_D} dk \frac{k^3}{e^{\beta \hbar c k} - 1} \\ &\simeq \frac{\partial}{\partial T} \frac{3(k_B T)^4}{2\pi^2 (\hbar c)^3} \underbrace{\int_0^\infty \frac{x^3}{e^x - 1} dx}_{\pi^4/15} = \frac{\partial}{\partial T} \frac{\pi^2 (k_B T)^4}{10 (\hbar c)^3} = \frac{2\pi^2}{5} k_b \left( \frac{k_B T}{\hbar c} \right)^3 \quad (84) \end{aligned}$$

So far we have done nothing which couldn't have been done easily by ordinary 1st-quantized methods. I have reviewed some Solid State I material here by way of introduction to problems of interacting particles to which you have not been seriously exposed thus far in the condensed matter grad sequence. The second quantization method becomes manifestly useful for the analysis of *interacting* systems. I will now sketch the formulation (not the solution) of the problem in the case of the phonon-phonon interaction in the anharmonic crystal.

#### 1.4.4 Anharmonicity & its consequences

As you will recall from Solid State I, most thermodynamic properties of insulators, as well as neutron scattering experiments on most materials, can be explained entirely in terms of the harmonic approximation for the ions in the crystal, i.e. by assuming a Hamiltonian of the form (80). There are some problems with the harmonic theory. First, at higher temperatures atoms tend to explore the anharmonic parts of the crystal potential more and more, so deviations from predictions of the equilibrium theory increase. The thermal expansion of solids in the harmonic approximation is rigorously zero.<sup>14</sup> Secondly, some important qualitative aspects of transport cannot be understood: for example, the harmonic theory predicts infinite thermal transport of insulators! (See A&M Ch. 25 for a qualitative discussion of these failures).

The obvious way to go beyond the harmonic approximation is to take into account higher-order corrections to the real-space crystal potential systematically, expanding<sup>15</sup>

$$U = \frac{1}{2!} \sum_{\ell m} D^{(2)}(\ell, m) q_\ell q_m + \frac{1}{3!} \sum_{\ell m n} D^{(3)}(\ell, m, n) q_\ell q_m q_n + \dots, \quad (86)$$

where

$$D^{(n)}(\ell, m, \dots n) = \left. \frac{\partial^n U}{\partial q_\ell \partial q_m \dots \partial q_n} \right|_{u_i=0} \quad (87)$$

---

<sup>14</sup>This follows from the independence of the phonon energies in harmonic approx. of the system volume. (see above) Since pressure depends on temperature only through the volume derivative of the mode freqs. (see A & M p. 490),

$$\left( \frac{\partial V}{\partial T} \right)_p = \frac{\left( \frac{\partial p}{\partial T} \right)_V}{\left( \frac{\partial p}{\partial V} \right)_T} = 0 \quad (85)$$

<sup>15</sup>I have dropped polarization indices everywhere in this discussion, so one must be careful to go back and put them in for a 2- or 3D crystal.

are the so-called dynamical matrices.<sup>16</sup> Using Eqs. (71,76) we find

$$q_\ell = \frac{1}{\sqrt{N}} \left( \frac{\hbar}{2m\omega} \right)^{1/2} \sum_k Q_k e^{ik\ell} = \sum_k (a_k + a_{-k}^\dagger) e^{ik\ell} \quad (88)$$

Note that the product of 3 displacements can be written

$$q_\ell q_m q_n = \frac{1}{(N)^{3/2}} \sum_{k_1 k_2 k_3} e^{i(k_1 \ell + k_2 m + k_3 n)} Q_{k_1} Q_{k_2} Q_{k_3} \quad (89)$$

so the cubic term may be written

$$H_3 = \sum_{k_1 k_2 k_3} V^{(3)}(k_1 k_2 k_3) Q_{k_1} Q_{k_2} Q_{k_3} \quad (90)$$

with

$$V^{(3)}(k_1 k_2 k_3) = \sum_{\ell m n} D^{(3)}(\ell, m, n) \exp[i(k_1 \ell + k_2 m + k_3 n)] \quad (91)$$

Note now that the indices  $\ell$ ,  $m$ ,  $n$  run over all unit cells of the crystal lattice. Since crystal potential itself is periodic, the momenta  $k_1$ ,  $k_2$ , and  $k_3$  in the sum are not really independent. In fact, if we shift all the sums in (91) by a lattice vector  $j$ , we would have

$$\begin{aligned} V^{(3)}(k_1 k_2 k_3) &= \sum_{\ell m n} D^{(3)}(\ell + j, m + j, n + j) e^{i(k_1 \ell + k_2 m + k_3 n)} e^{i(k_1 + k_2 + k_3)aj} \\ &= \sum_{\ell m n} D^{(3)}(\ell, m, n) e^{i(k_1 \ell + k_2 m + k_3 n)} e^{i(k_1 + k_2 + k_3)aj} \end{aligned} \quad (92)$$

where in the last step I used the fact that the crystal potential  $U$  in every lattice cell is equivalent. Now sum both sides over  $j$  and divide by  $N$  to find

$$V^{(3)}(k_1 k_2 k_3) = \sum_{\ell m n} D^{(3)}(\ell, m, n) \exp[i(k_1 \ell + k_2 m + k_3 n)] \Delta(k_1 + k_2 + k_3), \quad (93)$$

---

<sup>16</sup>Recall that the theory with only harmonic and cubic terms is actually formally unstable, since arbitrarily large displacements can lower the energy by an arbitrary amount. If the cubic terms are treated perturbatively, sensible answers normally result. It is usually better to include quartic terms as shown in figure below, however.

where

$$\Delta(k) = \frac{1}{N} \sum_j e^{i(k_1+k_2+k_3)aj} = \frac{1}{N} \sum_k \delta(k + G) \quad (94)$$

and  $G$  is any reciprocal lattice vector.

Return now to (90). We have ascertained that  $V^{(3)}(\ell, m, n)$  is zero unless  $k_1 + k_2 + k_3 = G$ , i.e. crystal momentum is conserved. If we expand (90), we will get products of 3 creation or annihilation operators with coefficients  $V^{(3)}$ . The values of these coefficients depend on the elastic properties of the solid, and are unimportant for us here. The momenta of the three operators must be such that momentum is conserved up to a reciprocal lattice vector, e.g. if we consider the term  $a_{k_1} a_{-k_2}^\dagger a_{-k_3}^\dagger$  we have a contribution only from  $k_1 + k_2 + k_3 = G$ .<sup>17</sup> Note this term should be thought of as corresponding to a physical process wherein a phonon with momentum  $k_1$  is destroyed and two phonons with momenta  $-k_2$  and  $-k_3$  are created. It can be drawn "diagrammatically" à la Feynman (as the 1st of 2 3rd-order processes in the figure below).

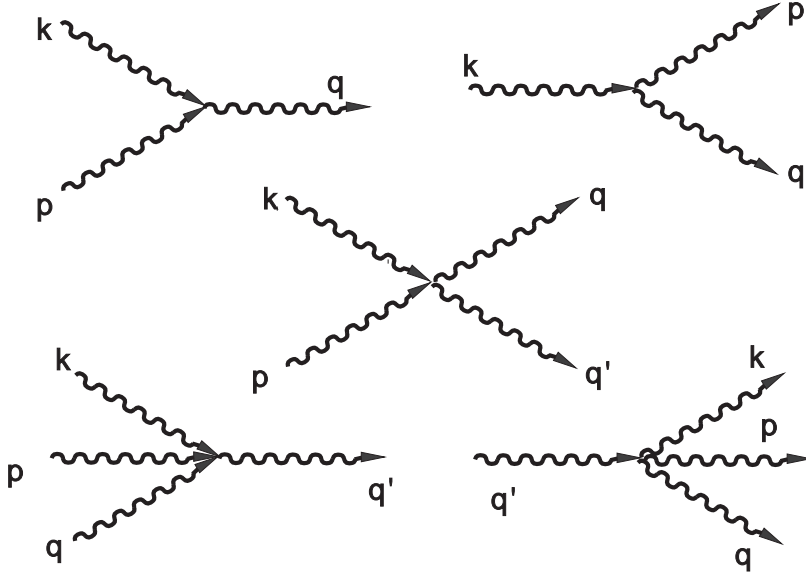


Figure 4: Diagrams representing phonon-phonon collision processes allowed by energy and momentum conservation in 3rd and 4th order.

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<sup>17</sup>As usual, processes with  $G = 0$  are called *normal* processes, and those with finite  $G$  are called *Umklapp* processes.

Questions:

- How does energy conservation enter? What is importance of processes involving destruction or creation of 3 phonons?
- If one does perturbation theory around harmonic solution, does cubic term contribute to thermal averages?
- Can we calculate thermal expansion with cubic Hamiltonian?

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## **Reading:**

1. Ch. 17, Ashcroft & Mermin
2. Chs. 5& 6, Kittel
3. For a more detailed discussion of Fermi liquid theory, see G. Baym and C. Pethick, Landau Fermi-Liquid Theory : Concepts and Applications, Wiley 1991

## **2 Electron-electron interactions**

The electronic structure theory of metals, developed in the 1930's by Bloch, Bethe, Wilson and others, assumes that electron-electron interactions can be neglected, and that solid-state physics consists of computing and filling the electronic bands based on knowledge of crystal symmetry and atomic valence. To a remarkably large extent, this works. In simple compounds, whether a system is an insulator or a metal can be determined reliably by determining the band filling in a noninteracting calculation. Band gaps are sometimes difficult to calculate quantitatively, but inclusion of simple renormalizations to 1-electron band structure known as Hartree-Fock corrections, equivalent to calculating the average energy shift of a single electron in the presence of an average density determined by all other electrons (“mean field theory”), almost always

suffices to fix this problem. There are two reasons why we now focus our attention on  $e^- - e^-$  interactions, and why almost all problems of modern condensed matter physics as it relates to metallic systems focus on this topic:

1. Why does the theory work so well in simple systems? This is far from clear. In a good metal the average interelectron distance is of the order of or smaller than the range of the interaction, e.g. the screening length  $\ell_{scr} \sim (c/e^2m)^{1/2}\rho^{-1/6}$ , where  $\rho$  is the density, of order 1nm for typical parameters. One might therefore expect that interactions should strongly modify the picture of free electrons commonly used to describe metals.
2. More complicated systems exhibit dramatic deviations from the predictions of band theory. I refer now not simply to large quantitative errors in the positions of 1-electron bands, but to qualitative discrepancies in the behavior of the materials. The most interesting modern example is the class of compounds known as the transition metal oxides, including the cuprate materials which give rise to high-temperature superconductivity (HTS).<sup>1</sup>

---

<sup>1</sup>The parent compounds of the HTS (e.g.  $\text{La}_2\text{CuO}_4$  and  $\text{YBa}_2\text{Cu}_3\text{O}_4$  are without exception *antiferromagnetic* and *insulating*. Historically, this discovery drove much of the fundamental interest in these materials, since standard electronic structure calculations predicted they should be paramagnetic metals. This can easily be seen by simple valence counting arguments. The nominal valences in e.g.  $\text{La}_2\text{CuO}_4$  are  $\text{La}^{3+}$ ,  $\text{O}^{2-}$ , and  $\text{Cu}^{2+}$ . The  $\text{La}$  and  $\text{O}$  ions are in closed shell configurations, whereas the  $\text{Cu}$  is in an  $[\text{Ar}]3d^9$  state, i.e. a single d-hole since

## 2.1 Mean field theory (Hartree-Fock)

Let's begin with the second-quantized form of the electronic Hamiltonian with 2-body interactions. The treatment will be similar to that of Kittel (Ch. 5), but for comparison I will focus on a translationally invariant system and do the calculation in momentum space. In this case as we have shown the Hamiltonian is<sup>2</sup>

$$\hat{H} = \hat{T} + \hat{V}, \quad (1)$$

$$\hat{T} = \sum_{\mathbf{k}\sigma} \left( \frac{\mathbf{k}^2}{2m} \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (2)$$

$$\hat{V} = \frac{1}{2\mathcal{V}} \sum_{\substack{\mathbf{k}, \mathbf{k}', \mathbf{q} \\ \sigma, \sigma'}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger V(\mathbf{q}) c_{\mathbf{k}'\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}. \quad (3)$$

The 2-body interaction  $\hat{V}$  contains 4 Fermi operators  $c$  and is therefore not exactly soluble. The goal is to write down an *effective* 2-body

---

there are 10 d electrons in a filled shell. The 1 hole/unit cell would then suggest a 1/2 filled band and therefore a metallic state. The crystal field splittings in the planar Cu environment give the  $3d_{x^2-y^2}$  state being lowest in energy (see later), and since the n.n.'s are the  $O$ 's, it would seem likely that the lowest  $O$  crystal field state in the planar environment, the  $O$   $3p$ , will hybridize with it. Sophisticated LDA calculations confirm this general picture that the dominant band at the Fermi level is a 1/2-filled planar  $Cu$   $d_{x^2-y^2}$ -  $O$   $3p$  band. Instead, this compound is found experimentally to be an electrical insulator and an antiferromagnet with a Neel temperature of 300K! This strongly suggests that the band calculations are missing an important element of the physics of the high- $T_c$  materials. In the transition metals and TMO's band theory is notoriously bad at calculating band gaps in insulators, because of the presence of strong local Coulomb interactions which lead to electronic correlations neglected in the theory. It is therefore reasonable to assume that a similar mechanism may be at work here: extremely strong Coulomb interactions in the  $Cu - O$  planes are actually opening up a gap in the 1/2-filled band at the Fermi level and simultaneously creating a magnetic state. This phenomenon has been studied in simpler systems since the 60s and is known as the *Mott-Hubbard* transition.

<sup>2</sup>For the moment, we ignore the ionic degrees of freedom and treat only the electrons. To maintain charge neutrality, we therefore assume the electrons move in a neutralizing positive background ("jellium model").

Hamiltonian which takes into account the average effects of the interactions. We therefore replace the 4-Fermi interaction with a sum of all possible 2-body terms,

$$c_1^\dagger c_2^\dagger c_3 c_4 \simeq -\langle c_1^\dagger c_3 \rangle c_2^\dagger c_4 - \langle c_2^\dagger c_4 \rangle c_1^\dagger c_3 + \langle c_1^\dagger c_4 \rangle c_2^\dagger c_3 + \langle c_2^\dagger c_3 \rangle c_1^\dagger c_4, \quad (4)$$

where the  $+$  and  $-$  signs are dictated by insisting that one factor of -1 occur for each commutation of two fermion operators required to achieve the given ordering. This can be thought of as “mean field terms”, in the spirit of Pierre Weiss, who replaced the magnetic interaction term  $S_i \cdot S_j$  in a ferromagnet by  $\langle S_i \rangle S_j = \langle S \rangle S_j \equiv -H_{eff} S_j$ , i.e. he replaced the field  $S_i$  by its homogeneous mean value  $S$ , and was left with a term equivalent to a 1-body term corresponding to a spin in an external field which was soluble. The mean field  $\langle S \rangle$  in the Weiss theory is the instantaneous average magnetization of all the other spins except the spin  $S_j$ , and here we attempt the same thing, albeit somewhat more formally. The “mean field”

$$\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma'} \rangle = \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \equiv n_{\mathbf{k}\sigma} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \quad (5)$$

is the average number of particles  $n_{\mathbf{k}\sigma}$  in the state  $\mathbf{k}\sigma$ , which will be weighted with the 2-body interaction  $V(\mathbf{q})$  to give the average interaction due to all other particles (see below).<sup>3</sup>

---

<sup>3</sup>Note we have not allowed for mean fields of the form  $\langle c^\dagger c^\dagger \rangle$  or  $\langle aa \rangle$ . These averages vanish in a normal metal due to number conservation, but will be retained in the theory of superconductivity.

With these arguments in mind, we use the approximate form (4) and replace the interaction  $\hat{V}$  in (3) by

$$\begin{aligned}
\hat{V}_{HF} &= \frac{1}{2} \sum_{\substack{\mathbf{k}\mathbf{k}'\mathbf{q} \\ \sigma\sigma'}} V(\mathbf{q}) \left[ -\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma'} \rangle c_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} - \langle c_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} \rangle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma'} + \right. \\
&\quad \left. + \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} \rangle c_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger c_{\mathbf{k}'\sigma'} + \langle c_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger c_{\mathbf{k}'\sigma'} \rangle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} \right] \\
&= - \sum_{\substack{\mathbf{k}\mathbf{q} \\ \sigma}} V(\mathbf{q}) \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} + V(0) \sum_{\substack{\mathbf{k}\mathbf{k}' \\ \sigma\sigma'}} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle c_{\mathbf{k}'\sigma'}^\dagger c_{\mathbf{k}'\sigma'} \\
&= \sum_{\mathbf{k}\sigma} \left( - \sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q}\sigma} V(\mathbf{q}) + nV(0) \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \tag{6}
\end{aligned}$$

where the total density  $n$  is defined to be  $n = \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}$ . Since this is now a 1-body term of the form  $\sum_{\mathbf{k}\sigma} \Sigma_{HF}(\mathbf{k}) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$ , it is clear the full Hartree-Fock Hamiltonian may be written in terms of a  $\mathbf{k}$ -dependent energy *shift*:

$$\hat{H}_{HF} = \sum_{\mathbf{k}\sigma} \left( \frac{\hbar^2 k^2}{2m} + \Sigma_{HF}(\mathbf{k}) \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \tag{7}$$

$$\Sigma_{HF}(\mathbf{k}) = \underbrace{- \sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q}\sigma} V(\mathbf{q})}_{Fock} + \underbrace{nV(0)}_{Hartree} \tag{8}$$

$$Fock \quad Hartree \tag{9}$$

Note the Hartree or *direct Coulomb* term, which represents the average interaction energy of the electron  $\mathbf{k}\sigma$  with all the other electrons in the system, is merely a constant, and as such it can be absorbed into a chemical potential. In fact it is seen to be divergent if  $V(q)$  represents the Coulomb interaction  $4\pi e^2/q^2$ , but this divergence must cancel exactly with the constant arising from the sum of the self-energy of the posi-

tive background and the interaction energy of the electron gas with that background.<sup>4</sup> The Fock, or *exchange* term<sup>5</sup> is a momentum-dependent shift.

### 2.1.1 Validity of Hartree-Fock theory

Crucial question: when is such an approximation a good one for an interacting system? The answer depends on the range of the interaction. The HF approximation becomes asymptotically exact *for certain quantities* in the limit of *high density* Fermi systems if interactions are sufficiently long-range! This is counterintuitive, for it seems obvious that if the particles are further apart on the average, they will interact less strongly and less often, so a mean field theory like Hartree-Fock theory should work well. This is true if the interactions are short-ranged, such that for sufficiently low densities the particles spend no time within an interaction length. The interaction is typically characterized by a *strength*  $V$  and a *range*  $a$ , and if the interparticle spacing  $r_0 \gg a$ , the particles don't feel the potential much and the ground state energy, for example, of such a gas can be expanded at  $T = 0$  in powers of  $a/r_0$ . If  $a \rightarrow 0$ , the interaction disappears and the the only characteristic en-

---

<sup>4</sup>See e.g., Kittel

<sup>5</sup>The origin of the term exchange is most easily seen in many-body perturbation theory, where the Fock term is seen to arise from a scattering process where the particle in state  $\mathbf{k}\sigma$  changes places with a particle from the medium in an intermediate state.

energy left at  $T = 0$  is the zero-point energy, i.e. the energy scale obtained by confining the particle to a cage of size the interparticle spacing  $r_0$ , i.e.  $\hbar^2/(2mr_0^2)$ . This is just the Fermi energy in the case of a Fermi system. Thus we might expect HF theory to be quite good for a dilute gas of  $^3\text{He}$ , since the  $^3\text{He}$ - $^3\text{He}$  interaction is certainly short-ranged; unfortunately, liquid  $^3\text{He}$  has  $a \simeq r_0$ , so corrections to HF are always important.

What about for a metal? We can do a simple argument to convince ourselves that HF isn't applicable for low density systems with Coulomb interactions. Let's rewrite the basic 2-body Hamiltonian in dimensionless variables,

$$\hat{H} = \sum_{\mathbf{k}\sigma} \left( \frac{\hbar^2 k^2}{2m} \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2\mathcal{V}} \sum_{\substack{\mathbf{k}, \mathbf{k}', \mathbf{q} \\ \sigma, \sigma'}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'+\mathbf{q}\sigma'}^\dagger \left( \frac{4\pi e^2}{q^2} \right) c_{\mathbf{k}'\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma} \quad (10)$$

$$= \frac{e^2}{2a_0 r_s^2} \left( \sum_{\bar{\mathbf{k}}\sigma} \bar{k}^2 c_{\bar{\mathbf{k}}\sigma}^\dagger c_{\bar{\mathbf{k}}\sigma} + \frac{3r_s}{N} \sum_{\substack{\bar{\mathbf{k}}, \bar{\mathbf{k}}', \bar{\mathbf{q}} \\ \sigma, \sigma'}} c_{\bar{\mathbf{k}}\sigma}^\dagger c_{\bar{\mathbf{k}}'+\bar{\mathbf{q}}\sigma'}^\dagger \left( \frac{1}{\bar{q}^2} \right) c_{\bar{\mathbf{k}}'\sigma'} c_{\bar{\mathbf{k}}+\bar{\mathbf{q}}\sigma} \right) \quad (11)$$

where I've used the system volume  $\mathcal{V} = N(4/3)\pi r_0^3$ , Bohr radius  $a_0 = \hbar^2/me^2$ , defined  $r_s \equiv r_0/a_0$ , and scaled all momenta as  $\mathbf{k} = \bar{\mathbf{k}}r_0^{-1}$ , etc. Applying dimensional analysis, we expect the two terms  $\sum \bar{k}^2 c^\dagger c$  and  $\sum c^\dagger c^\dagger (1/\bar{q}^2) c c$  to be of order 1, so that it is clear that the interaction term becomes negligible in the limit  $r_s \rightarrow 0$  (high density). On the

other hand, it's also clear that had the  $1/q^2$  factor not been present in the interaction, it would have scaled as  $1/r_s$  instead, and become negligible in the low density limit.

One can do a more careful, formal perturbation analysis for a simple quantity like the ground state energy  $\langle H \rangle$  of the electron gas, which is discussed in many-body physics texts. The result is

$$E_0 = E_0^{HF} + E_{corr} \quad (12)$$

with  $E_0^{HF}$  the ground state energy calculated in the independent particle approximation with the Hartree-Fock energy shifts, and  $E_{corr}$  the *correlation energy*, defined to be the part of the g.s. energy not captured by HF. As the density increases, so does  $\varepsilon_F$ , which represents the average kinetic energy per electron; this increase is faster than the increase of the correlation energy, as

$$K.E. = \frac{3}{5}\varepsilon_F = \frac{2.21}{r_s^2} \text{ Ryd} \quad (13)$$

$$P.E.|_{HF} = \frac{-0.916}{r_s} \text{ Ryd} \quad (14)$$

$$E_{corr} = (0.0622 \log r_s - 0.096 + \dots) \text{ Ryd} \quad (15)$$

so it is clear the correlation term is less singular than the HF term in the limit  $r_s \rightarrow 0$ . At higher densities, particles are effectively independent.<sup>6</sup>

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<sup>6</sup>For a more detailed discuss of these terms, see Fetter & Wallecka, *Quantum Theory of Many-Particle Systems*

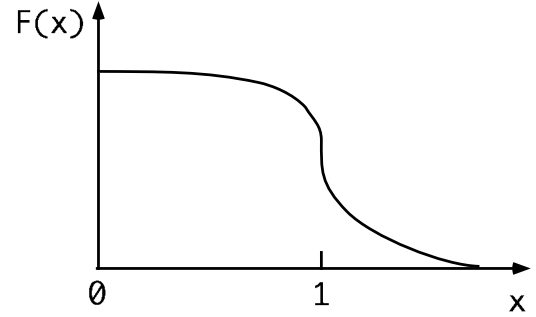


### 2.1.2 Problem with Hartree-Fock theory

Although we argued that the Hartree-Fock approximation becomes a better approximation in the limit of high density for electrons interacting via the Coulomb interaction, it never becomes exact, as one can see by examining the Fourier transform of the Hartree-Fock energy shift. The Hartree term itself (being  $\mathbf{k}$  independent) is absorbed into a redefinition of the chemical potential, so the shift is (T=0):

$$\delta\varepsilon_{\mathbf{k}} = \pm \frac{1}{L^3} \sum_{|\mathbf{k}'| < k_F} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2} \quad (16)$$

$$= \frac{2e^2 k_F}{\pi} F(k/k_F), \quad (17)$$



where  $F(x)$  is a function which has a log divergence in slope at  $x = 1$ , i.e. at the Fermi level.<sup>7</sup> This means while the energy *shift* might be small compared to the Fermi energy  $\mathbf{v}\varepsilon_F$ , the *velocity* of an electron is  $\partial\varepsilon_{\mathbf{k}}/\partial\mathbf{k}|_{k_F}$ , which contains a term which is infinite.

---

<sup>7</sup>The integral is straightforward & useful:

$$\frac{1}{L^3} \sum'_{\mathbf{k}'} \frac{1}{(\mathbf{k} - \mathbf{k}')^2} = \int_0^{k_F} \frac{k^2 dk}{4\pi^2} \int_{-1}^1 dx \frac{1}{k^2 - k'^2 - 2kk'x} = \frac{1}{8\pi^2 k} \int_0^{k_F} dk' k' \log \left| \frac{k + k'}{k - k'} \right| \quad (18)$$

$$= \frac{1}{8\pi^2} \left( \frac{k_F^2 - k^2}{k} \log \left| \frac{k_F + k}{k_F - k} \right| + 2k_F \right) \quad (19)$$

so with  $z = k/k_F$  and (17) we have

$$\boxed{F(z) = \frac{1 - z^2}{4z} \log \left| \frac{1 + z}{1 - z} \right| + \frac{1}{2}} \quad (20)$$

This problem can be traced back to the long-range nature of the Coulomb force. Two electrons at large distances  $\mathbf{r} - \mathbf{r}'$  don't really feel the full  $1/|\mathbf{r} - \mathbf{r}'|^2$  but a “screened” version due to the presence of the intervening medium, i.e. The electron gas rearranges itself to cancel out the long-range part of  $V$ .

## 2.2 Screening

### 2.2.1 Elementary treatment

To see how this works, let's first examine the problem of a single fixed (i.e. infinite mass) charge placed inside an electron gas. We are interested in how the electron gas responds to this perturbation (recall in the HF approximation the perturbation would simply be the interaction of the charge with the uniform gas). But since the electrons are mobile and negatively charged, they will tend to cluster around the test charge if its charge is positive, and be repelled (i.e. have a lower density) around the test charge if it is negative. In addition, Fermi statistics lead to long-range *oscillations* of the electron charge density far from the test charge.

This is not entirely a “Gedanken experiment”. Impurities in solids may have different valences from the host, and thus acquire a localized

charge, although the entire solid is still neutral. As an example of some relevance to modern condensed matter physics, consider what happens when you put an extra Oxygen atom in the  $\text{CuO}_2$  plane of a cuprate high- $T_c$  superconducting material. Although the crystal structure of these materials is complex, they all contain  $\text{CuO}_2$  planes as shown in the figures. The interstitial oxygen will capture two electrons from the valence band, changing it from a  $2s^2 2p^4$  to a  $2s^2 2p^6$  electronic configuration. The impurity will then have a net charge of two electrons. For  $\mathbf{r}$

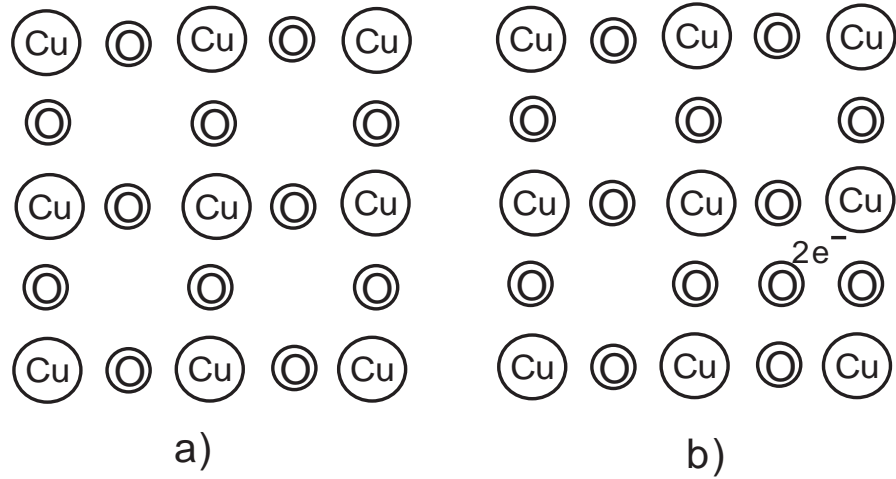


Figure 1: a) The  $\text{CuO}_2$  plane of cuprate superconductor. b) Interstitial charged O impurity.

near the impurity, the electronic charge density will be reduced by the Coulomb interaction. The electronic number density fluctuation is<sup>8</sup>

$$n(\mathbf{r}) \approx \int_{-e\delta\phi(\mathbf{r})}^{\varepsilon_F} N(\omega + e\delta\phi(\mathbf{r}))d\omega \approx \int_0^{\varepsilon_F + e\delta\phi(\mathbf{r})} N(\omega')d\omega' \quad (21)$$

---

<sup>8</sup>A note on signs: the electrostatic potential  $\delta\phi(\mathbf{r}) < 0$  due to the excess negative charge at the impurity. You might worry about this: the total change in  $\phi$  should include the self-consistently determined positive charge screening the impurity. We have fudged this a bit, and the correct separation between induced and external quantities will become clear later in the discussion. Note we take  $e > 0$  always, so the electron has charge  $-e$ .

Note that this equation involves the double-spin density of states, which we will use throughout this section. On the other hand, in the bulk far

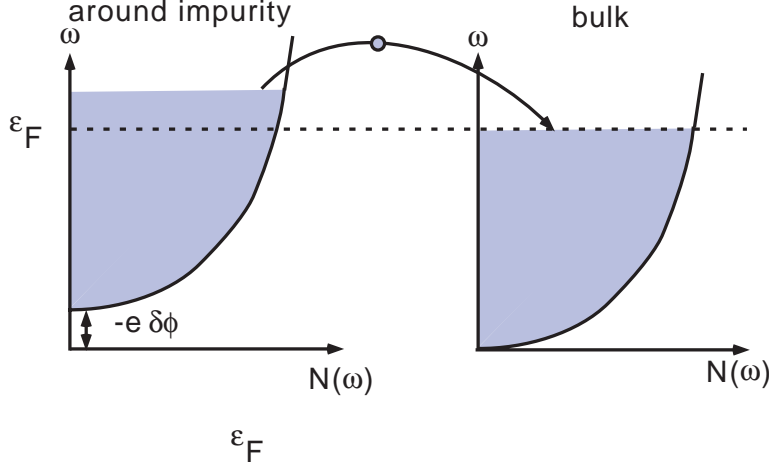


Figure 2: *Local repulsion of charge due to shift of electronic density of states near impurity*

away from the impurity,  $\delta\phi(\mathbf{r}_{bulk}) = 0$ , so

$$n(\mathbf{r}_{bulk}) \approx \int_0^{\epsilon_F} N(\omega) d\omega \quad (22)$$

or

$$\delta n(\mathbf{r}) \approx \int_0^{\epsilon_F + e\delta\phi(\mathbf{r})} N(\omega) d\omega - \int_0^{\epsilon_F} N(\omega) d\omega \quad (23)$$

Let us assume a *weak potential*  $|e\delta\phi| \ll \epsilon_F$ ; therefore

$$\delta n(\mathbf{r}) \approx N(\epsilon_F) [\epsilon_F + e\delta\phi - \epsilon_F] = +e\delta\phi N_0. \quad (24)$$

We can solve for the change in the electrostatic potential by solving Poisson's equation.

$$\nabla^2 \delta\phi = -4\pi\delta\rho = 4\pi e\delta n = 4\pi e^2 N_0 \delta\phi. \quad (25)$$

Define a new length  $k_{TF}^{-1}$ , the Thomas-Fermi screening length, by  $k_{TF}^2 = 4\pi e^2 N_0$ , so that P's eqn. is  $\nabla^2 \delta\phi = r^{-2} \partial_r r^2 \partial_r \delta\phi = k_{TF}^2 \delta\phi$ , which has

the solution  $\delta\phi(\mathbf{r}) = C \exp(-k_{TF}r)/r$ . Now  $C$  may be determined by letting  $N(\varepsilon_F) = 0$ , so the medium in which the charge is embedded becomes vacuum. Then the potential of the charge has to approach  $q/r$ , so  $C = q$ , i.e. in the electron gas

$$\delta\phi(\mathbf{r}) = \frac{qe^{-k_{TF}r}}{r}, \quad (26)$$

where  $q = -2e$  for our example.

Let's estimate some numbers, by using the free electron gas. Use  $k_F = (3\pi^2n)^{1/3}$ ,  $a_0 = \hbar^2/(me^2) = 0.53\overset{\circ}{\text{\AA}}$ , and  $N(\varepsilon_F) = mk_F/(\hbar^2\pi^2)$ . Then we find

$$\begin{aligned} k_{TF}^{-2} &= \frac{a_0\pi}{4(3\pi^2n)^{1/3}} \approx \frac{a_0}{4n^{1/3}} \\ k_{TF}^{-1} &\approx \frac{1}{2} \left( \frac{n}{a_0^3} \right)^{-1/6} \end{aligned} \quad (27)$$

In Cu, for which  $n \approx 10^{23} \text{ cm}^{-3}$  (and since  $a_0 = 0.53\overset{\circ}{\text{\AA}}$ )

$$k_{TF}^{-1} \approx \frac{1}{2} \frac{(10^{23})^{-1/6}}{(0.5 \times 10^{-8})^{-1/2}} \approx 0.5 \times 10^{-8} \text{ cm} = 0.5\overset{\circ}{\text{\AA}} \quad (28)$$

Thus, if we add a charged impurity to Cu metal, the effect of the impurity's ionic potential is exponentially screened away for distances  $r > \frac{1}{2}\overset{\circ}{\text{\AA}}$ . The screening length in a semiconductor can clearly be considerably longer because  $n$  is much smaller, but because of the  $1/6$  power which appears in, even with  $n = 10^{-10}$ ,  $k_{TF}^{-1}$  is only about 150 times larger or  $75\overset{\circ}{\text{\AA}}$ .

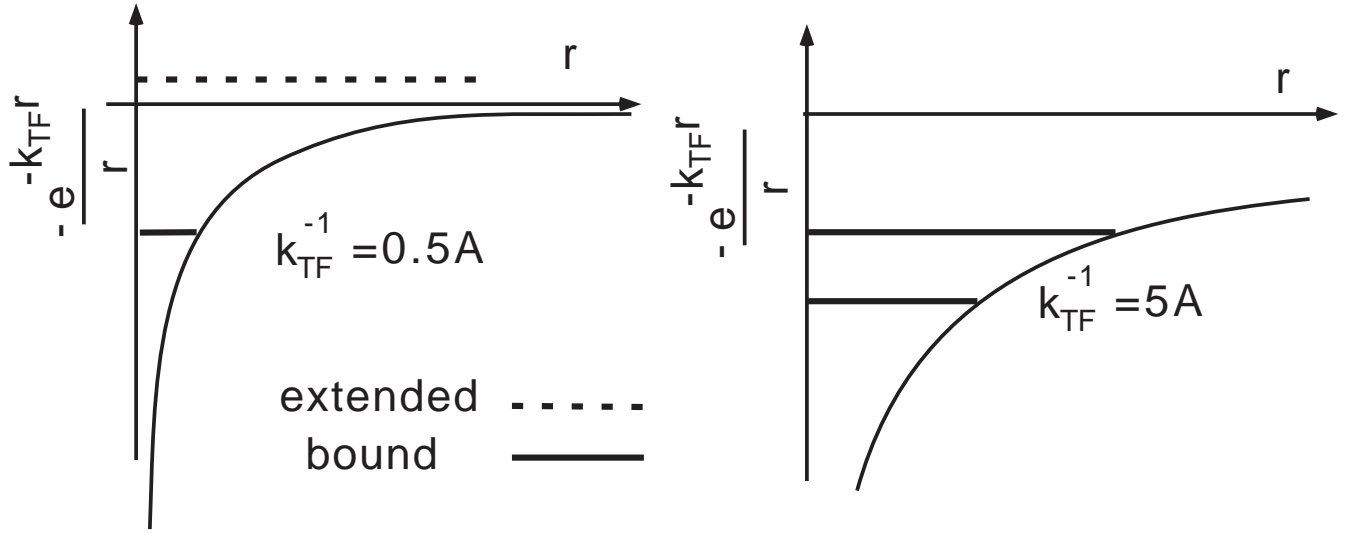


Figure 3: *Screened impurity potentials. As the density decreases, the screening length increases, so that states which were extended bound.*

What happens in the quantum-mechanical problem of an electron moving in the potential created by the impurity when the screening length gets long? As shown in the figure, the potential then correspondingly deepens, and from elementary quantum mechanics we expect it to be able to bind more electrons, i.e bound states “pop out” of the continuum into orbits bound to the impurity site.

In a poor metal (e.g., YBCO), in which the valence state is just barely unbound, decreasing the number of carriers will increase the screening length, since

$$k_{TF}^{-1} \sim n^{-1/6}. \quad (29)$$

This will extend the range of the potential, causing it to trap or bind more states—making the one free valence state bound. Of course, this

has only a small effect  $\mathcal{O}(1/N)$  effect on the bulk electrical properties of the material. Now imagine that instead of a single impurity, we have a concentrated system of such ions, and suppose that we decrease  $n$  (e.g. in Si-based semiconductors, this is done by adding acceptor dopants, such as B, Al, Ga, etc.). This will in turn, increase the screening length, causing some states that were free to become bound, eventually possibly causing an abrupt transition from a metal to an insulator. This process is believed to explain the metal-insulator transition in some amorphous semiconductors.

### 2.2.2 Kubo formula

Many simple measurements on bulk statistical systems can be described by applying a small external probe field of some type to the system at  $t = 0$ , and asking how the system responds. If the field is small enough, the response is proportional to the external perturbation, and the proportionality constant, a *linear response coefficient*, is given always in terms of a *correlation function* of the system in the equilibrium ensemble without the perturbation. In Table 1 I list some standard linear response coefficients for condensed matter systems.

System	Perturbation	Response	Coefficient
metal	electric field $\mathbf{E}$	current $\mathbf{j}$	conductivity $\sigma$
	temp. gradient $\nabla T$	heat current $\mathbf{j}_Q$	thermal cond. $\kappa$
	point charge $q$	density fluct. $\delta n$	density correlation function $\chi_c$
	magnetic field $B$	magnetization $M$	susceptibility $\chi_s$

The general theory of linear response is embodied in the *Kubo formula*.<sup>9</sup> Suppose a perturbation  $\hat{H}'(t)$  is turned on at time  $t = 0$ . The idea is to express the subsequent time-dependence of expectation values of physical observables in terms of matrix elements of the perturbation *in the unperturbed ensemble*. The unperturbed ensemble is described by  $\hat{H}_0$ , which may involve interactions, but is usually assumed to be time-independent. All observables can be calculated by knowing the time evolution of the statistical operator  $\rho(t)$ , given by the Heisenberg equation

$$i\frac{\partial \hat{\rho}}{\partial t} = [\hat{H}_0 + \hat{H}', \hat{\rho}] \quad (30)$$

First one defines a canonical transformation<sup>10</sup>:

$$\tilde{\rho}(t) = \hat{S}(t)\hat{\rho}(t)\hat{S}^\dagger; \quad S(t) \equiv e^{i\hat{H}_0 t} \quad (31)$$

---

<sup>9</sup>R. Kubo, J. Phys. Soc. Jpn. 12, 570 (1957).

<sup>10</sup>The idea is to remove the “trivial” time-evolution of  $\hat{\rho}$  on  $\hat{H}$ , to isolate the dependence on  $\hat{H}'$ .



from which one can see by substituting into (30) that

$$i\frac{\partial\tilde{\rho}}{\partial t} = [\tilde{H}', \tilde{\rho}] \quad (32)$$

with  $\tilde{H}' = \hat{S}\hat{H}'\hat{S}^\dagger$ . This has the formal solution

$$\tilde{\rho}(t) = \tilde{\rho}(0) - i \int_0^t [\tilde{H}', \tilde{\rho}(0)] dt'. \quad (33)$$

The initial condition is  $\tilde{\rho}(0) = \hat{S}(0)\hat{\rho}(0)\hat{S}(0)^\dagger = \hat{\rho}(0)$ , and we can iterate the rhs by substituting  $\hat{\rho}(0)$  for  $\tilde{\rho}(0)$ , etc.<sup>11</sup> Since we are interested only in leading order, we write

$$\tilde{\rho}(t) \simeq \hat{\rho}(0) - i \int_0^t [\tilde{H}', \hat{\rho}(0)] dt'. \quad (34)$$

If we now multiply on the left by  $\hat{S}^\dagger$  and on the right by  $\hat{S}$ , we obtain the leading order in  $\hat{H}'$  change in the original  $\rho$ :

$$\hat{\rho}(t) \simeq \hat{\rho}(0) - i\hat{S}^\dagger(t) \left\{ \int_0^t [\tilde{H}', \hat{\rho}(0)] dt' \right\} \hat{S}(t), \quad (35)$$

which can now be used to construct averages in the usual way. The expectation value of an operator  $\hat{\mathcal{O}}$  at nonzero  $T$  and at some time  $t$  is

$$\langle \hat{\mathcal{O}} \rangle \equiv \text{Tr}(\hat{\rho}(t)\hat{\mathcal{O}}) \quad (36)$$

$$\begin{aligned} &\simeq \text{Tr}(\hat{\rho}(0)\hat{\mathcal{O}}) - i \int dt' \text{Tr}(\hat{S}^\dagger(t)[\tilde{H}', \hat{\rho}(0)]\hat{S}(t)\hat{\mathcal{O}}) \\ &= \text{Tr}(\hat{\rho}(0)\hat{\mathcal{O}}) - i \int dt' \text{Tr}(\hat{\rho}(0)[\tilde{H}', \hat{\mathcal{O}}_H(t)]), \end{aligned} \quad (37)$$

---

<sup>11</sup>Note  $\hat{\rho}(0)$  is the unperturbed but still interacting density matrix (statistical operator). I reserve the symbol  $\hat{\rho}_0$  for the noninteracting analog.

where in the last step the cyclic property of the trace and the definition of the Heisenberg operator  $\hat{O}_H = \hat{S}\hat{O}\hat{S}^\dagger$  was used. The change in the expectation value due to the perturbation is then

$$\boxed{\delta\langle\hat{\mathcal{O}}\rangle = -i \int dt' \text{Tr} \left( \hat{\rho}(0) [\tilde{H}', \hat{\mathcal{O}}_H(t)] \right)} \quad (38)$$

Since typically  $\hat{H}'$  is proportional to some external (c-number) field, we can write  $\hat{H}'$  as  $\hat{H}'(t) = \int d^3r \hat{B}(\mathbf{r})\phi(\mathbf{r}, t)$  (so  $\tilde{H}'(t) = \int d^3r \hat{B}_H(\mathbf{r}, t)\phi(\mathbf{r}, t)$ ), and

$$\delta\langle\hat{A}(1)\rangle = -i \int_0^t \int \text{Tr} \left( \hat{\rho}(0) [\hat{A}_H(1), \hat{B}_H(1')] \right) \phi(1') d1' \quad (39)$$

$$\equiv \int_0^\infty G_{AB}(1, 1') \phi(1') d1'. \quad (40)$$

with the notation  $1 \equiv \mathbf{r}, t, \sigma$ ,  $1' = \mathbf{r}', t', \sigma'$ ,  $\int d1' \equiv \sum_{\sigma'} \int d^3r' dt'$ , etc.<sup>12</sup>

### 2.2.3 Correlation functions

As a concrete example, consider the change in the density  $\delta n(\mathbf{r}, t)$  of a system in response to a local change in its density perhaps at a different place and time  $\delta n(\mathbf{r}', t')$ , where  $\hat{n}(\mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \rangle$ , and  $\langle \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \rangle_{\hat{H}'=0} = n_0$ . It's usually convenient to set  $n_0 = 0$ , i.e. we assume an overall neutral system. The linear response function is then

$$\chi(\mathbf{r}, t; \mathbf{r}', t') = -i \langle [\hat{n}(\mathbf{r}, t), \hat{n}(\mathbf{r}', t')] \rangle_{\hat{H}'=0} \theta(t - t'), \quad (41)$$

---

<sup>12</sup>The object  $\text{Tr} \left( \hat{\rho}(0) [\hat{A}_H(1), \hat{B}_H(1')] \right)$  which appears on the right-hand side of (38) is related to something called a retarded 2-particle Green's function, which I have promised not to oppress you with.

where the expectation value is taken in the unperturbed system. The function  $G_{nn}$  measures the average amplitude in the unperturbed ensemble a particle is to be found at  $\mathbf{r}', t'$  and subsequently at  $\mathbf{r}, t$ . If the particles are statistically independent,  $\chi$  factorizes,  $\langle nn' \rangle \sim \langle n \rangle \langle n' \rangle = 0$  (no *correlations*), so it has the interpretation of a *correlation function*.

### 2.2.4 Dielectric constant

The simplest way to analyze this problem conceptually is to ask what is the potential a long distance from a test charge placed into the interacting electron gas medium. This potential will be the sum of the bare potential produced by the test charge in a vacuum, plus the induced potential due to the polarization of the medium.

Let's use what we learned about linear response in the last section to calculate the electric potential in the system  $\phi(\mathbf{r}, t)$  due to an *external* potential  $\phi^{ext}(\mathbf{r}', t')$  (you may think of this as the potential due to a test charge if you like). From electrodynamics we recall these two are supposed to be proportional, and that the proportionality constant is just the dielectric constant  $\epsilon$ . By analogy we write, in Fourier transformed language,

$$\phi^{ext}(\mathbf{q}, \omega) = \epsilon(\mathbf{q}, \omega) \phi(\mathbf{q}, \omega) \quad (42)$$

It is the dielectric constant of the medium (which is directly related to

the conductivity) which we now wish to calculate.

The total potential in the material is the sum of the external potential and the induced potential,

$$\phi = \phi^{ind} + \phi^{ext}, \quad (43)$$

but in fact we can calculate the induced potential  $\phi^{ind}$  by

- first finding the induced change in density  $\delta\rho^{ind}$  due to the external potential, using linear response theory; then
- using Poisson's equation to calculate the induced electric potential.

The additional term in the Hamiltonian in the presence of the “test charge” is

$$\hat{H}' = e \int d^3r \, \hat{n}(\mathbf{r}) \phi(\mathbf{r}, t) \quad (44)$$

where  $\hat{n}$  is the 2nd-quantized density operator  $\hat{\psi}^\dagger \hat{\psi}$ . The induced change in charge density  $\delta\rho = e\langle\hat{n}\rangle$  is then just given by the Kubo formula as above,<sup>13</sup>

$$\delta\rho^{ind}(1) = -ie^2 \int_0^t \int d^3r' \text{Tr}(\hat{\rho}(0)[\hat{n}_H(1), \hat{n}_H(1')]) \phi^{ext}(1') d1' \quad (45)$$

$$\equiv e^2 \int_0^\infty \chi(1, 1') \phi^{ext}(1') d1' \quad (46)$$

where the density-density correlation function is<sup>14</sup>

$$\chi(1, 1') = -i \text{Tr}(\hat{\rho}(0)[\hat{n}_H(1), \hat{n}_H(1')]) \theta(t - t'). \quad (47)$$

---

<sup>13</sup>Don't confuse charge density  $\rho$  with statistical operator  $\hat{\rho}$ .

<sup>14</sup>Instead of  $G_{nn}^{(2)}$ , it's more conventional to use the notation  $\chi_{nn}$  or just  $\chi$ .

For a translationally invariant system in Fourier transform rep., the convolution (46) reduces to

$$\delta\rho^{ind}(\mathbf{q}, \omega) = e^2\chi(\mathbf{q}, \omega)\phi^{ext}(\mathbf{q}, \omega). \quad (48)$$

Now using Poisson's equation  $q^2\phi^{ind} = 4\pi\delta\rho^{ind}$ , and Eq. (43), we find<sup>15</sup>

$$\phi^{ind}(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2}\chi(\mathbf{q}, \omega)\phi^{ext}(\mathbf{q}, \omega) \equiv V(\mathbf{q})\chi(\mathbf{q}, \omega)\phi^{ext} \quad (49)$$

so

$$\epsilon(\mathbf{q}, \omega) \equiv \frac{\phi^{ext}(\mathbf{q}, \omega)}{\phi^{ind}(\mathbf{q}, \omega) + \phi^{ext}(\mathbf{q}, \omega)} = \frac{1}{1 + V(\mathbf{q})\chi(\mathbf{q}, \omega)}. \quad (50)$$

### 2.2.5 Lindhard function

We've found the exact structure of the dielectric response,<sup>16</sup> but not really solved it because we still don't know the density-density correlation function  $\chi$ . For the interacting system this can be a very difficult problem, but it is not too hard to find it for the free fermion gas. We will need

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<sup>15</sup>Compare Eq. (25)

<sup>16</sup>Warning! Compare the treatment here with e.g., A& M pp. 337-340, and you will see that they arrive at the apparently different result

$$\epsilon(\mathbf{q}, \omega) = 1 - V(\mathbf{q})\chi(\mathbf{q}, \omega), \quad (51)$$

which is also claimed to be exact. This is because  $\chi$  is defined to be the response to the total potential

$$\rho^{ind}(\mathbf{q}, \omega) = \chi|_{A\&M}(\mathbf{q}, \omega)\phi(\mathbf{q}, \omega) \quad (52)$$

which is very difficult to calculate since  $\phi$  is self-consistently determined.

- The definitions of Fourier transforms

$$\begin{aligned}
\chi(\mathbf{q}, \omega) &= \int d^3(\mathbf{r} - \mathbf{r}') \int d(t - t') e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\omega(t - t')} \chi(1, 1') \\
c_{\mathbf{k}}^\dagger(t) &= \int d^3r e^{i\mathbf{k} \cdot \mathbf{r}} \hat{\psi}^\dagger(1) \\
c_{\mathbf{k}}(t) &= \int d^3r e^{-i\mathbf{k} \cdot \mathbf{r}} \hat{\psi}(1)
\end{aligned} \tag{53}$$

- the integral expression for the theta function

$$\theta(t - t') = - \int \frac{d\omega'}{2\pi i} \frac{e^{-i\omega'(t - t')}}{\omega' + i\eta^+}, \tag{54}$$

where  $\eta^+$  is a positive infinitesimal.<sup>17</sup>

- the solutions of the Heisenberg equation of motion  $i\partial_t \hat{\mathcal{O}}_H(t) = [\hat{\mathcal{O}}_H(t), H]$  for  $c_{\mathbf{k}\sigma}^\dagger(t)$  and  $c_{\mathbf{k}\sigma}(t)$  for free fermions (check):

$$c_{\mathbf{k}\sigma}^\dagger(t) = c_{\mathbf{k}\sigma}^\dagger e^{i\epsilon_{\mathbf{k}} t} \tag{55}$$

$$c_{\mathbf{k}\sigma}(t) = c_{\mathbf{k}\sigma} e^{-i\epsilon_{\mathbf{k}} t} \tag{56}$$

- The commutator (check!)

$$[c_{k_1}^\dagger c_{k_2}, c_{k_3}^\dagger c_{k_4}] = \delta_{k_2 k_3} c_{k_1}^\dagger c_{k_4} - \delta_{k_1 k_4} c_{k_3}^\dagger c_{k_2} \tag{57}$$

- The expectation values in the noninteracting ensemble of the number operator at finite temperature  $T$  are

$$\langle \hat{n}_{\mathbf{k}} \rangle = f(\epsilon_{\mathbf{k}}), \tag{58}$$

where  $f$  is the Fermi function.

---

<sup>17</sup>The sign of the infinitesimal is important. It determines in which complex half-plane the contour can be completed to evaluate the integral by Cauchy's theorem. Check it!

Then (supressing spin indices)

$$\begin{aligned}
\langle [n_H(1), n_H[1']] \rangle &= \text{Tr}(\hat{\rho}_0[n_H(1), n_H[1']]) \\
&= \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} e^{i(\mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}'} \langle [c_{\mathbf{k}_1}^\dagger(t) c_{\mathbf{k}_2}(t), c_{\mathbf{k}_3}^\dagger(t') c_{\mathbf{k}_4}(t')] \rangle \\
&= \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} e^{i(\mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}'} e^{i([\epsilon_{\mathbf{k}_3} - \epsilon_{\mathbf{k}_4}]t' + [\epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_2}]t)} \langle [c_{\mathbf{k}_1}^\dagger c_{\mathbf{k}_2}, c_{\mathbf{k}_3}^\dagger c_{\mathbf{k}_4}] \rangle \\
&= \sum_{\mathbf{k}_1 \mathbf{k}_2} e^{i(\mathbf{k}_1 \cdot [\mathbf{r} - \mathbf{r}'] + \mathbf{k}_2 \cdot [\mathbf{r}' - \mathbf{r}])} e^{i(\epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_1})(t' - t)} \langle \hat{n}_{\mathbf{k}_2} \rangle \\
&\quad - \sum_{\mathbf{k}_3 \mathbf{k}_4} e^{i(\mathbf{k}_4 \cdot [\mathbf{r} - \mathbf{r}'] + \mathbf{k}_3 \cdot [\mathbf{r}' - \mathbf{r}])} e^{i(\epsilon_{\mathbf{k}_3} - \epsilon_{\mathbf{k}_4})(t' - t)} \langle \hat{n}_{\mathbf{k}_4} \rangle
\end{aligned} \tag{59}$$

so that (using (47) and (53), and putting back the spin sum)

$$\boxed{\chi_0(\mathbf{q}, \omega) = \sum_{\mathbf{k}\sigma} \frac{f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}+\mathbf{q}})}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta}}. \tag{60}$$

This is the so-called Lindhard function, the charge susceptibility of the free Fermi gas. Note that in the free gas the major contributions to the integral (60) come from contributions where  $\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \omega = 0$ . These correspond to 2-particle “particle-hole excitations” where the Fermi sea is given a little energy  $\omega$  which promotes a particle from below the Fermi surface (say  $\mathbf{k}$ ) to above (say  $\mathbf{k} + \mathbf{q}$ ). In the homework you will investigate when such excitations are possible within this model.

The use of the free gas susceptibility  $\chi_0$  for  $\chi$  in Eq. (50) is a rather poor approximation, as it completely ignores the effect of the long-range Coulomb interaction on the intermediate states. The self-consistent field method, or random phase approximation, replaces the induced charge

without interactions with the screened charge:

$$\chi_0 \equiv \left. \frac{\rho^{ind}}{\phi^{ext}} \right|_{V=0} \rightarrow \frac{\rho^{ind}|_{V=0}/\epsilon}{\phi^{ext}} = \frac{\chi_0}{\epsilon}. \quad (61)$$

Solving (50) for  $\epsilon$  gives

$$\boxed{\epsilon(\mathbf{q}, \omega) \simeq 1 - V(\mathbf{q})\chi_0(\mathbf{q}, \omega)} \quad (RPA/SCF) \quad (62)$$

This is sometimes called the Lindhard approx. to the dielectric function.

### 2.2.6 Thomas-Fermi theory

Let us consider the static limit of the theory we currently have. This will allow us to answer the original question we posed: if we insert a charge somewhere into a metal, what is the net electrostatic potential felt at some distance  $r$  away by a second charge? Taking the  $\omega \rightarrow 0$  limit in (60), we find

$$\chi_0(\mathbf{q}, 0) = \sum_{\mathbf{k}\sigma} \frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}}) - f(\varepsilon_{\mathbf{k}})}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + i\eta^+} \quad (63)$$

First note that if we further take the limit  $q \rightarrow 0$  we find (recall  $N_0$  is double-spin dos!)

$$\chi_0 \rightarrow -2 \sum_k \frac{-\partial f}{\partial \varepsilon_{\mathbf{k}}} \simeq -N_0 \int d\xi_{\mathbf{k}} \underbrace{\frac{-\partial f}{\partial \xi_{\mathbf{k}}}}_{T \ll \epsilon_F} \simeq -N_0 \int d\xi_{\mathbf{k}} \delta(\xi_{\mathbf{k}}) = -N_0. \quad (64)$$



The dielectric constant in the long-wavelength (i.e. small  $q$ ) limit may thus be written

$$\epsilon(q, 0) \simeq 1 + \frac{4\pi e^2}{q^2} N_0 \equiv 1 + \frac{k_{TF}^2}{q^2}, \quad (65)$$

where  $k_{TF}$  is the same Thomas-Fermi wave vector  $k_{TF}^2 \equiv 4\pi e^2 N_0$  we discussed earlier. Now we go back: if we had placed a charge  $e$  in a vacuum, it would have produced a potential  $\phi^{ext}(r) = e/r$ , or  $\phi^{ext}(q) = 4\pi e/q^2$  everywhere in space. From (42) we see that the actual potential in the medium is

$$\phi(q) = \phi^{ext}(q)/\epsilon(q) = \frac{4\pi e/q^2}{1 + k_{TF}^2/q^2} = \frac{4\pi e}{k_{TF}^2 + q^2}, \quad (66)$$

i.e. the Thomas-Fermi wavevector *cuts off* the divergence of the bare long-range Coulomb interaction. In real space

$$\boxed{\phi(\mathbf{r}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \phi(\mathbf{q}) = \frac{e}{r} e^{-k_{TF}r}}, \quad (67)$$

so the long-range interaction is indeed replaced by an exponentially cut off short-range one, with *screening length* scale  $k_{TF}^{-1}$ .

### 2.2.7 Friedel oscillations

The Thomas-Fermi theory is very intuitive and describes realistically how the singularities of the long-range Coulomb interaction are cut off by screening. It suffices to eliminate the anomalies encountered in Hartree-Fock theory of transport and density of states near the Fermi level. But

because it is a long-wavelength approximation, it cannot describe adequately the response of the electron gas to a short-range perturbation. Our initial example of a point charge placed in an electron gas was just such a case. To get an accurate description of the screened impurity potential, the finite- $q$  dependence of the charge susceptibility must be accounted for. This calculation involves simply replacing our Thomas-Fermi dielectric function  $\varepsilon_{TF} = 1 - k_{TF}^2/q^2$  with the expression involving the full Lindhard function

$$\varepsilon_{Lindhard} = 1 - V(q)\chi_0(q, \omega = 0) = 1 - \frac{k_{TF}^2}{q^2} F\left(\frac{q}{2k_F}\right), \quad (68)$$

where  $F$  is the same function as in (20). Then we repeat the same calculation for the impurity potential

$$\phi(\mathbf{r}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{\phi^{ext}(\mathbf{q})}{1 - \frac{k_{TF}^2}{q^2} F\left(\frac{q}{2k_F}\right)} \simeq \frac{x^2}{(2 + x^2)^2} \frac{\cos 2k_F r}{r^3}, \quad (69)$$

where  $x = k_{TF}/(2k_F)$ . The main interesting feature of this result is of course the fact that the potential no longer has the simple Yukawa form with exponential decay, but in fact an *oscillatory*  $1/r^3$  behavior. The last step in (69) is a bit long,<sup>18</sup> but I have attempted to give you a flavor of it in the homework. One of the main conclusions of the exercise there is that the potential is very sensitive to the details of the charge susceptibility at  $2k_F$ , which the Thomas-Fermi theory clearly

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<sup>18</sup>See e.g. Fetter & Walecka

gets wrong. Ultimately Friedel oscillations (and RKKY oscillations, their counterpart for magnetic spins) originate from the sharpness of the Fermi surface.

### 2.2.8 Plasmons

An examination of the dielectric function of the solid, e.g. Eq. (50), shows that the dielectric function can be zero, meaning the system responds very strongly to a small perturbation (see Eq. (42). These are the excitation energies of the electron gas. In the random phase approximation (62) this means there are excitations when

$$V(\mathbf{q})\chi_0(\mathbf{q}, \omega) = 1 \quad (70)$$

Consider first a finite size box where the energy levels  $\epsilon_{\mathbf{k}}$  are discrete. This means  $\chi_0(\mathbf{q}, \omega)$  is a sum of terms containing simple poles at the particle-hole excitation energies  $\omega_{\mathbf{q}}(\mathbf{k}) \equiv \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}$ .  $\chi_0$  will change sign and diverge as  $\omega$  passes through these energies, therefore there will be a solution of (70) for each excitation energy. It is simplest to focus on the limit at  $T = 0$ , where

$$\sum_{\substack{k < k_F \\ |\mathbf{k}+\mathbf{q}| > k_F}} \left\{ \frac{1}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{1}{\omega - (\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}) + i\eta} \right\} \quad (71)$$

In other words, the poles in the complex  $\omega$  plane are particle-hole excitation energies  $\pm\omega_{\mathbf{k}}(\mathbf{q}) \equiv \xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}$ , where  $|\mathbf{k} + \mathbf{q}|$  is always above

Fermi surface and  $\mathbf{k}$  always below.<sup>19</sup> The situation is depicted in figure 4. At  $T = 0$ , there is a maximum frequency above which there are no

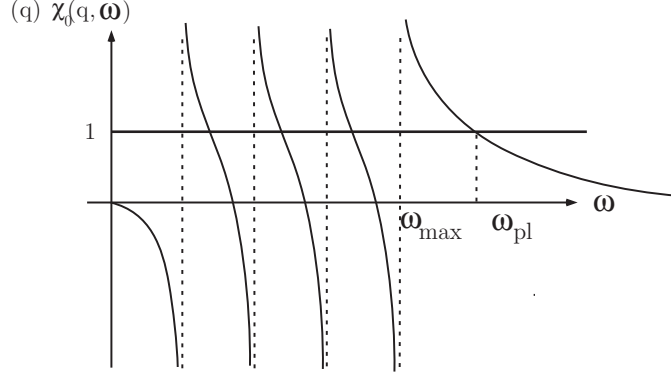


Figure 4: Eigenfrequencies of electron gas in RPA.

more particle-hole excitations possible for given fixed  $q$ , i.e. the largest excitation energy occurs when  $k = k_F$  and  $\mathbf{k}, \mathbf{q}$  are parallel, so that for a parabolic band,  $\epsilon_{\mathbf{k}} = k^2/(2m)$ ,

$$\omega_{max} = \frac{k_F q}{m} + \frac{q^2}{2m}. \quad (72)$$

---

<sup>19</sup>To arrive at this result, note from (60)

$$\begin{aligned}
\chi_0(\mathbf{q}, \omega) &= \sum_{\mathbf{k}} \frac{f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}+\mathbf{q}})}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} = \\
&= \sum_{\mathbf{k}} \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}})) - f(\xi_{\mathbf{k}+\mathbf{q}})(1 - f(\xi_{\mathbf{k}}))}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} = \\
&= \sum_{\mathbf{k}} \left\{ \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}}))}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{f(\xi_{\mathbf{k}+\mathbf{q}})(1 - f(\xi_{\mathbf{k}}))}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} \right\} \\
&= \sum_{\mathbf{k}} \left\{ \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}}))}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}-\mathbf{q}}))}{\omega - (\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}}) + i\eta} \right\} \\
&= \sum_{\mathbf{k}} \left\{ \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}}))}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{f(\xi_{-\mathbf{k}})(1 - f(\xi_{-\mathbf{k}-\mathbf{q}}))}{\omega - (\xi_{-\mathbf{k}} - \xi_{-\mathbf{k}-\mathbf{q}}) + i\eta} \right\} \\
&= \sum_{\mathbf{k}} \left\{ \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}}))}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}}))}{\omega - (\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}) + i\eta} \right\} \\
&= \sum_{\mathbf{k}} f(\xi_{\mathbf{k}})(1 - f(\xi_{\mathbf{k}+\mathbf{q}})) \left\{ \frac{1}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{1}{\omega - (\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}) + i\eta} \right\} \\
\lim_{T \rightarrow 0} &= \sum_{\substack{k < k_F \\ |\mathbf{k}+\mathbf{q}| > k_F}} \left\{ \frac{1}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{1}{\omega - (\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}) + i\eta} \right\}
\end{aligned}$$

There is another possible root of  $\epsilon$ , as also shown in Fig. (4). In the limit  $\omega > \omega_{max}$ , we may expand (71) for small  $q$ , and find

$$\begin{aligned}\chi(\mathbf{q}, \omega) &\simeq -\frac{2q^2}{m\omega^2} \sum_{k < k_F} \left[ 1 + \frac{2\mathbf{k} \cdot \mathbf{q}}{m\omega} + 3 \left( \frac{\mathbf{k} \cdot \mathbf{q}}{m\omega} \right)^2 + \dots \right] \\ &\simeq -\frac{k_F^3}{3\pi^2} \frac{q^2}{m\omega^2} \left[ 1 + \frac{3}{5} \left( \frac{k_F q}{m\omega} \right)^2 + \dots \right].\end{aligned}\quad (73)$$

Now we look for a solution to  $\text{Re}V\chi_0 = 1$  and find to leading order<sup>20</sup>

$$\omega = \omega_{pl} \left( 1 + \mathcal{O}(q/k_F)^2 + \dots \right), \quad (74)$$

with

$$\omega_{pl} = \left( \frac{4\pi n e^2}{m} \right)^{1/2} \quad (75)$$

which is of course the plasma frequency you found by elementary methods last semester. In contrast to the particle-hole excitations, which involve exciting only 1 particle from its position in the Fermi sea, a plasma oscillation perforce involves motions of all particles and is therefore referred to as a collective mode of the system. Plasmons have been observed indirectly in metals, primarily in thin metallic films.

## 2.3 Fermi liquid theory

In a good metal the average interelectron distance is of the order of or smaller than the range of the interaction, e.g. the screening length

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<sup>20</sup>Note this is a result for 3 dimensions. It is a useful exercise to obtain the analagous result for 2D, which has  $\omega \sim q^{1/2}$ , i.e a gapless mode.

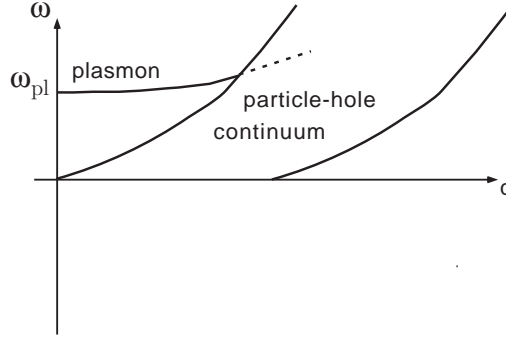


Figure 5: Excitations (poles of  $\epsilon(\mathbf{q}, \omega)^{-1}$ ) at  $T = 0$ .

$k_{TF}^{-1} \approx 0.5 (n/a_0^3)^{-1/6}$ , where  $n$  is the density, of order 0.1-1nm for typical parameters. One might therefore expect that interactions should strongly modify the picture of free electrons commonly used to describe metals. It turns out, however, that for  $T \ll T_F$  the important degrees of freedom are mostly frozen out, and only a fraction  $T/T_F$  of all electrons near the Fermi surface participate in interaction processes. This leads to the possibility of a mapping between the free Fermi gas and the interacting Fermi system. If the elementary excitations of the many-body system can be obtained from the single-particle states of the free electron gas by turning on the interaction adiabatically (and if the ground state has the full symmetry of the Hamiltonian), the distribution function  $n_{k\sigma}$  of the interacting system would be the same as that of a free gas, and the particle and hole excitations of the gas would evolve into “quasiparticle” and “quasi-hole” states.

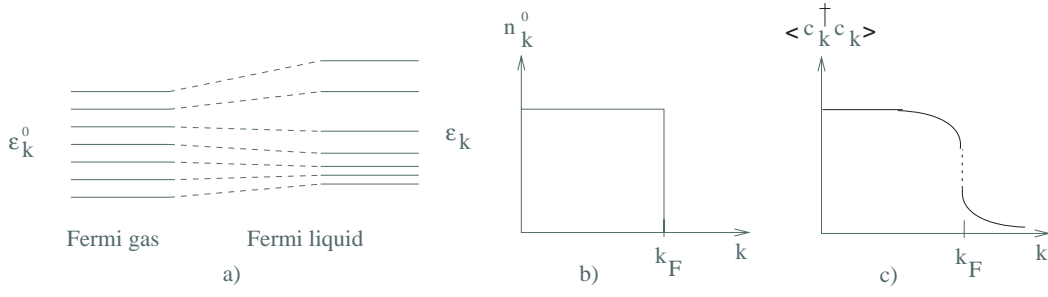


Figure 6: a) Evolution of quasiparticle states; b)  $T = 0$  Quasiparticle distribution function  $n_k^0$ ; c)  $T = 0$  true electron distribution function  $\langle c_k^\dagger c_k \rangle$ .

### 2.3.1 Particles and holes

To understand what this really means, let's go back and review the definitions of the terms particles and holes. Let's take  $N$  free Fermions, mass  $m$  in a volume  $L^3$ , where we know that the eigenstates are Slater determinants of  $N$  different single particle states, each given by

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (76)$$

Let's stick to  $T = 0$  for the moment, and recall that the occupation of each state is given by  $n_{\mathbf{k}} = \theta(k - k_F)$ , where  $k_F$  is the radius ermi sea.

Now let's add one “test” particle to the lowest available state  $k = k_F$ .

We then have for the chemical potential at  $T = 0$ ,

$$\mu = E_0(N + 1) - E_0(N) = \frac{\partial E_0}{\partial N} = \frac{k_F^2}{2m}. \quad (77)$$

Particles and holes are excitations of the filled Fermi sea. Excitations of the gas consist of taking a certain number of particles and moving them to the other side of the Fermi surface, yielding particles above and an

equal number of holes below the Fermi surface. These excitations can be described in terms of the changes in the particle occupation numbers  $\delta n_p = n_p - n_p^0$ :

$$\delta n_k = \begin{cases} \delta_{k,k'} & \text{for a particle } k' > k_F \\ -\delta_{k,k'} & \text{for a hole } k' < k_F \end{cases} . \quad (78)$$

At nonzero temperatures, a thermal fluctuation will create changes in

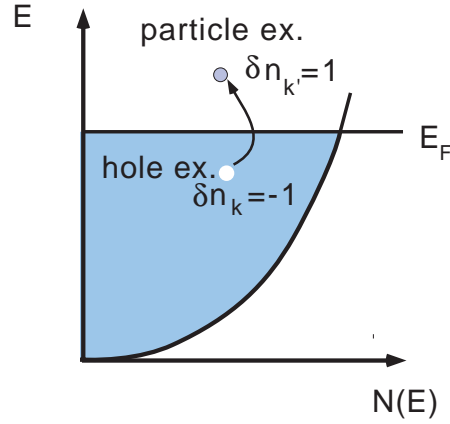


Figure 7: *Particle and hole excitations of the Fermi gas.*

occupation numbers  $\delta n_p \sim 1$  only for excitations of energy within  $k_B T$  of  $\varepsilon_F$ . Note that the total energy of the free gas is completely specified as a functional of the occupation numbers:

$$E - E_0 = \sum_{\mathbf{k}} \frac{k^2}{2m} (n_k - n_k^0) = \sum_{\mathbf{k}} \frac{k^2}{2m} \delta n_k . \quad (79)$$

Now take the gas and put it in contact with a particle reservoir. The appropriate thermodynamic potential is then the Gibbs free energy,



which for  $T = 0$  is  $F = E - \mu N$ , and

$$F - F_0 = \sum_{\mathbf{k}} \left( \frac{k^2}{2m} - \mu \right) \delta n_{\mathbf{k}} \equiv \sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}}. \quad (80)$$

The free energy of one particle, with momentum  $\mathbf{k}$  and occupation  $\delta n_{\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'}$  is  $\xi_{\mathbf{k}}$  and it corresponds to an excitation outside the Fermi surface. The free energy of a hole  $\delta n_{\mathbf{k}'} = -\delta_{\mathbf{k},\mathbf{k}'}$  is  $-\xi_{\mathbf{k}}$ , which corresponds to an excitation below the Fermi surface. For both species then the free energy of an excitation is  $|\xi_{\mathbf{k}}|$ , which is always positive; ie., the Fermi gas is stable with respect to excitations as it must be.

Quasiparticles and quasiholes in interacting system

Consider a system with interacting particles an average spacing  $a$  apart, so that the typical interaction energy is  $\frac{e^2}{a} e^{-a/r_{TF}}$ . As discussed above, we now suppose that we can create this system by turning on the interactions adiabatically starting from the free gas in a time  $t$ , such that the system evolves while staying always in its ground state.

If a state of the ideal system is characterized by the distribution  $n_{\mathbf{k}}^0$ , then the state of the interacting system will evolve adiabatically from  $n_{\mathbf{k}}^0$  to  $n_{\mathbf{k}}$ . In fact if the system remains in its ground state, then  $n_{\mathbf{k}}^0 = n_{\mathbf{k}}$ , i.e. the occupation of each state labelled by  $\mathbf{k}$  won't change (although the energy will). This is an assumption, and we will be studying some counterexamples to this ansatz (superconductivity and magnetism). But in general Landau expected this to hold if the *symmetry* of the interacting

system was the same as the noninteracting one, and this appears to be the case for simple metals.

Let's follow what happens to a particle of momentum  $\mathbf{k}$  added to the top of the non-interacting Fermi gas when we slowly turn the interaction knob. As  $U$  increases, two things happen. The  $\mathbf{k}$  state of the

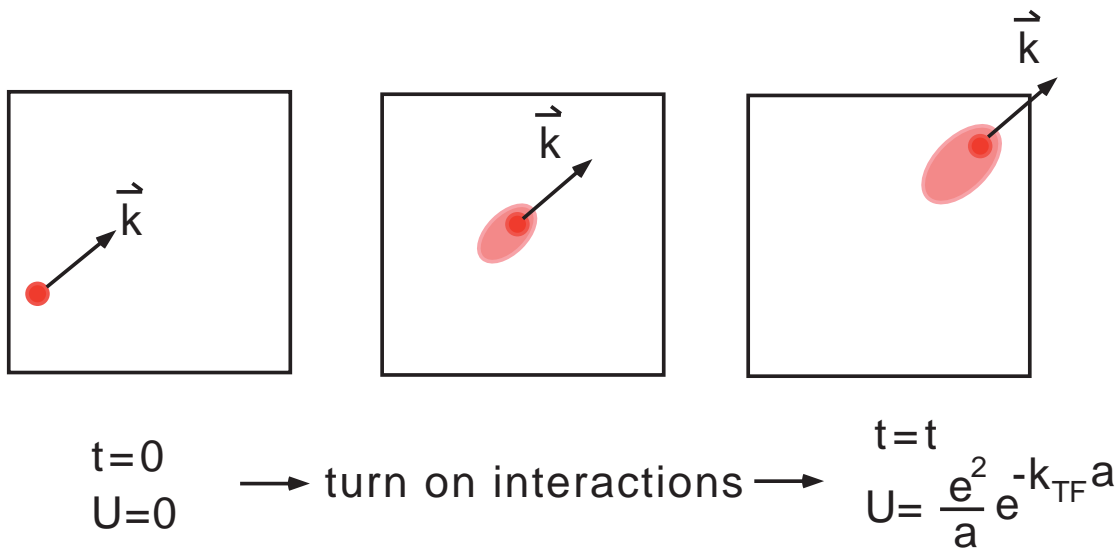


Figure 8: *Evolution of particle in state  $\mathbf{k}$  on top of Fermi sea as interaction is turned on. Particle becomes “dressed” by interactions with the rest of the system which changes the effective mass but not the momentum of the excitation (“quasiparticle”).*

original particle is no longer an eigenstate of  $\mathcal{H}$ , so it decays into the new excitations of the system, which according to our ansatz are also single-particle-like. Nearby particles also decay into the original state; this mixing has the effect of “dressing” the original free particle with a “cloud” of excitations of the surrounding system. However since momentum is conserved, the net excitation (called a *quasiparticle*)) can still be labelled with original momentum  $\mathbf{k}$ . In the same way, holes of

momentum  $\mathbf{k}$  below the Fermi surface evolve into quasiholes. Occasionally an analogy from classical mechanics is useful: we think of a bullet being fired into a large container filled with cotton. It will drag some cotton with it, and create a “particle+cloud” with increased mass but the same momentum.

It is too much to hope that the interactions between quasiparticles will vanish altogether. The  $N$ -particle ground state wave-function may still be Slater-determinant like, but this doesn’t necessarily imply that the quasiparticles are infinitely long-lived (exact) eigenstates of the system. So if each quasiparticle state  $\mathbf{k}$  has lifetime  $\tau_{\mathbf{k}}$ , we have to worry a bit about the adiabatic switching on procedure if  $\tau_{\mathbf{k}} < t$ . If so, the quasiparticle will decay before we finish switching, and we won’t be able to go reversibly back and forth. If we decrease  $t$  too much so again  $\tau_{\mathbf{k}} \gg t$ , then the switching on of  $U$  may not be adiabatic, i.e. we may knock the system into a state other than its ground state. It was Landau’s great insight to recognize that these objections are overcome for quasiparticle states sufficiently close to the Fermi energy. In this case the Pauli principle strongly restricts the decay channels for a quasiparticle, and one can argue (see below) that the lifetime becomes infinite at the Fermi energy itself. Therefore for any time  $t$  there should be a narrow range of energies near the Fermi surface for which the  $\tau_{\mathbf{k}}$  is long

enough to make the whole construction work.

### 2.3.2 Energy of quasiparticles.

As in the free gas, excitations will be characterized only by the deviation of the occupation number from the ground state occupation  $n_{\mathbf{k}}^0$ .<sup>21</sup>

$$\delta n_{\mathbf{k}} = n_{\mathbf{k}} - n_{\mathbf{k}}^0. \quad (81)$$

At sufficiently low temperatures  $\delta n_{\mathbf{k}} \sim 1$  only for those excitations near the Fermi surface where the condition  $\tau_{\mathbf{k}} \gg t$  is satisfied. Therefore we should be able to formulate a theory which depends only on  $\delta n_{\mathbf{k}}$ , not on  $n_{\mathbf{k}}$  or  $n_{\mathbf{k}}^0$ , which are not well defined for  $\mathbf{k}$  far from the Fermi surface.  $n_{\mathbf{k}}$  and  $n_{\mathbf{k}}^0$  should never enter independently and are not physically relevant.

For the noninteracting system the dependence of the energy ( $T = 0$ )  $E$  on  $\delta n_{\mathbf{k}}$  is very simple:

$$E - E_0 = \sum_{\mathbf{k}} \frac{k^2}{2m} \delta n_{\mathbf{k}}. \quad (82)$$

In the interacting case  $E[n_{\mathbf{k}}]$  is more complicated generally, but if we take  $\delta n_{\mathbf{k}}$  to be small (just a few excitations above the ground state) then we may expand:

$$E[n_{\mathbf{k}}] = E_o + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k}} + \mathcal{O}(\delta n_{\mathbf{k}}^2), \quad (83)$$

---

<sup>21</sup>Note we will now take over the notation  $n_{\mathbf{k}}^0$  which in the previous discussion meant the distribution function of the noninteracting system. Now it means the ground state of the interacting system. They are the same by Landau's ansatz.

where we now *define*  $\epsilon_{\mathbf{k}} = \delta E / \delta n_{\mathbf{k}}$ . If  $\delta n_{\mathbf{k}} = \delta_{\mathbf{k}, \mathbf{k}'}$ , then  $E \approx E_0 + \epsilon_{\mathbf{k}'}$ ; i.e., the energy of the quasiparticle with momentum  $\mathbf{k}'$  is  $\epsilon_{\mathbf{k}'}$ .

As discussed, we will only need  $\epsilon_{\mathbf{k}}$  near the Fermi surface where  $\delta n_{\mathbf{k}}$  is  $\mathcal{O}(1)$ . So we may expand  $\epsilon_{\mathbf{k}}$  around the Fermi level,

$$\epsilon_{\mathbf{k}} \approx \mu + (\mathbf{k} - \mathbf{k}_F) \cdot \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}|_{k_F} \quad (84)$$

where  $\nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} = v_{\mathbf{k}}$ , the group velocity of the quasiparticle. We no longer know the exact form of  $\epsilon_{\mathbf{k}}$ , but some exact relations must be obeyed because our system obeys certain symmetries. If we explicitly put the spin-dependence back in, we have symmetries

$$\epsilon_{\mathbf{k}, \sigma} = \epsilon_{-\mathbf{k}, -\sigma} \quad \text{time-reversal} \quad (85)$$

$$\epsilon_{\mathbf{k}, \sigma} = \epsilon_{-\mathbf{k}, \sigma} \quad \text{parity} \quad (86)$$

So unless we explicitly break  $T$ -symmetry by e.g. applying a magnetic field, we have  $\epsilon_{\mathbf{k}, \sigma} = \epsilon_{-\mathbf{k}, \sigma} = \epsilon_{\mathbf{k}, -\sigma}$ . Furthermore, as usual  $\epsilon_{\mathbf{k}}$  has to respect the point and space group symmetries of the system, e.g. for an isotropic system  $\epsilon_{\mathbf{k}}$  depends only upon the magnitude of  $\mathbf{k}$ ,  $|\mathbf{k}|$ , so  $\mathbf{k}$  and  $v_{\mathbf{k}} = \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}(|\mathbf{k}|) = \hat{k}(d\epsilon_k/dk)$  are parallel.<sup>22</sup> Define  $(m^*)^{-1}$  as the constant of proportionality at the Fermi surface<sup>23</sup>

$$v_{k_F} = k_F / m^* \quad (87)$$

---

<sup>22</sup>For a cubic system  $\epsilon_{\mathbf{k}}$  is invariant under  $90^\circ$  rotations, etc.

<sup>23</sup>Note  $k_F$  is not changed by interactions (Luttinger's theorem for isotropic system)

Then for the interacting system at the Fermi surface

$$N_{interacting}(\varepsilon_F) = \frac{m^* k_F}{\pi^3}, \quad (88)$$

the same *form* as for the noninteracting system. Note the  $m^*$  (usually but not always  $> m$ ) accounts for the dressing of the quasiparticle particle (bullet + cotton!). In other words, as far as the density of levels at the Fermi energy is concerned, the only thing which changes is the effective mass of the fermionic single-particle excitations.

### 2.3.3 Residual quasiparticle interactions

Let's go back to the Gibbs free energy of our system of quasiparticles characterized in some generalized excited state by distribution function  $\delta n_{\mathbf{k}}$ :

$$F - F_0 = E - E_0 - \mu(N - N_0). \quad (89)$$

where again  $F_0$ ,  $E_0$  etc. characterize the ground state. Thus,

$$N - N_0 = \sum_{\mathbf{p}} \delta n_{\mathbf{k}}, \quad (90)$$

and since

$$E - E_0 \approx \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k}} + \mathcal{O}(\delta n^2), \quad (91)$$

we get

$$F - F_0 \approx \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) \delta n_{\mathbf{k}} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}} + \mathcal{O}(\delta n^2). \quad (92)$$

As shown in Fig. 9, we will be interested in excitations of the system which deform the Fermi surface by an amount proportional to  $\delta$ . For example, along the positive  $k_x$  axis, our excited system has  $\delta n_{\mathbf{k}} = 1$  for some states  $\mathbf{k}$  above  $k_F$ , whereas along the negative  $k_x$  axis some states have  $\delta n_{\mathbf{k}} = -1$ . The approximation to the free energy above will

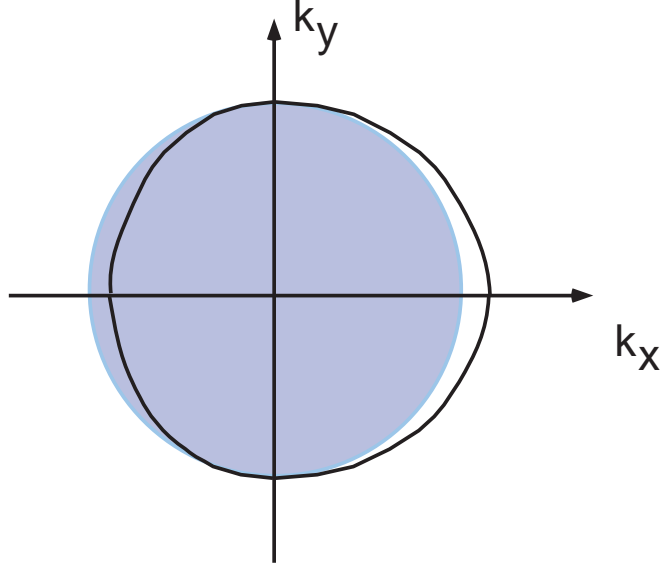


Figure 9: *Small deformations of the Fermi sphere, proportional to  $\delta$ .*

remain valid provided

$$\frac{1}{N} \sum_{\mathbf{k}} |\delta n_{\mathbf{k}}| \ll 1. \quad (93)$$

If we stick with our original criterion of using only states near the Fermi surface to construct our distortion, the  $\xi_{\mathbf{k}}$  for those states with  $\delta n_{\mathbf{k}} \neq 0$  will also be of order  $\delta$ . Thus,

$$\sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}} \sim \mathcal{O}(\delta^2), \quad (94)$$

so in order to keep terms of order  $\delta^2$  consistently we must also add the next term in the Taylor series expansion of the energy :

$$\boxed{F - F_0 = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} f_{\mathbf{k}, \mathbf{k}'} \delta n_{\mathbf{k}} \delta n_{\mathbf{k}'} + \mathcal{O}(\delta^3)} \quad (95)$$

where

$$f_{\mathbf{k}, \mathbf{k}'} = \frac{\delta E}{\delta n_{\mathbf{k}} \delta n_{\mathbf{k}'}} \quad (96)$$

The term proportional to  $f_{\mathbf{k}, \mathbf{k}'}$ , was proposed by L.D. Landau. It describes the residual interactions of the quasiparticle excitations which remain even after they are “dressed”. A glance at the dimensions of the new term shows that  $f_{\mathbf{k}, \mathbf{k}'} \sim 1/V$ . But if  $f_{\mathbf{k}, \mathbf{k}'}$  is an interaction between quasiparticles, each of which (in plane-wave like state) is delocalized over the whole volume  $V$ , so the probability that two will interact is roughly  $\sim k_{TF}^{-3}/V$ . Therefore

$$\boxed{f_{\mathbf{k}, \mathbf{k}'} \sim k_{TF}^{-3}/V} \quad (97)$$

We can proceed as earlier with the quasiparticle energy  $\epsilon_{\mathbf{k}}$  and ask how this unknown interaction function reflects the underlying symmetries of the physical system. To this end we reintroduce the hidden spin degrees of freedom. First in the absence of an external magnetic field, the system should be invariant under time-reversal, so

$$f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} = f_{-\mathbf{k}-\sigma, -\mathbf{k}'-\sigma'} , \quad (98)$$



and, in a system with reflection symmetry (parity)

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f_{-\mathbf{k}\sigma,-\mathbf{k}'\sigma'} . \quad (99)$$

Then since this implies

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f_{\mathbf{k}-\sigma,\mathbf{k}'-\sigma'} . \quad (100)$$

it must be that  $f$  depends only upon the relative orientations of the spins  $\sigma$  and  $\sigma'$ , so there are only two independent components for given  $\mathbf{k}, \mathbf{k}'$ , e.g.  $f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow}$  and  $f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow}$ . It is more conventional to decompose  $f$  into spin-symmetric and antisymmetric parts:

$$f_{\mathbf{k},\mathbf{k}'}^a = \frac{1}{2} (f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow} - f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow}) \quad f_{\mathbf{k},\mathbf{k}'}^s = \frac{1}{2} (f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow} + f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow}) . \quad (101)$$

$f_{\mathbf{k},\mathbf{k}'}^a$  may be interpreted as an exchange interaction, or

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f_{\mathbf{k},\mathbf{k}'}^s + \boldsymbol{\sigma} \cdot \boldsymbol{\sigma}' f_{\mathbf{k},\mathbf{k}'}^a \quad (102)$$

where  $\boldsymbol{\sigma}$  and  $\boldsymbol{\sigma}'$  are the Pauli matrices for the spins.

The next important assumption entering Fermi liquid theory is that the quasiparticle interactions are short-ranged. This means that  $f_{kk'}$  is essentially constant as a function of  $|\vec{k}|, |\vec{k}'|$ , and so depends only on the directions  $\hat{k}, \hat{k}'$ ,  $f_{kk'}^{s,a} \simeq f(\hat{k}, \hat{k}')$ :

$$f_{\mathbf{k},\mathbf{k}'} \simeq f_{\mathbf{k},\mathbf{k}'}|_{\epsilon_{\mathbf{k}}=\epsilon_{\mathbf{k}'}=\mu} \quad (103)$$

or equivalently, only on the angle  $\theta$  between them!

$$f_{\mathbf{k},\mathbf{k}'}^\alpha = \sum_{l=0}^{\infty} f_l^\alpha P_l(\cos \theta). \quad (104)$$

Conventionally these  $f$  parameters are expressed in terms of dimensionless quantities.

$$V N_0 f_l^\alpha = \frac{V m^* k_F}{\pi^2 \hbar^3} f_l^\alpha = F_l^\alpha. \quad (105)$$

We expect that the *Landau parameters*  $F_\ell^{s,a}$  will be negligible for sufficiently large  $\ell$ , so we have now achieved our goal of subsuming the complicated effects of interactions in a few phenomenological parameters.

### 2.3.4 Local energy of a quasiparticle

Now consider an interacting system with a certain distribution of excited quasiparticles  $\delta n_{\mathbf{k}'}$ . Let's add another particle, say of momentum  $\mathbf{k}$  and see how the energy changes. The distribution function goes from  $(\delta n'_{\mathbf{k}} \rightarrow \delta n'_{\mathbf{k}} + \delta_{\mathbf{k},\mathbf{k}'})$ . From Eq. 95 the free energy of the additional quasiparticle is

$$\tilde{\xi}_k = \xi_{\mathbf{k}} + \sum_{\mathbf{k}'} f_{\mathbf{k}',\mathbf{k}} \delta n_{\mathbf{k}'}, \quad (106)$$

(since  $f_{\mathbf{k}',\mathbf{k}} = f_{\mathbf{k},\mathbf{k}'}$ ). The second term on the right corresponds to the average interaction of a quasiparticle with the other quasiparticles in the

system.<sup>24</sup>

Substituting (104) and (105) in (106) gives the shift in energy of a quasiparticle due to the Landau interaction

$$\delta\xi_{\mathbf{k}\sigma} \equiv \tilde{\xi}_k - \xi_{\mathbf{k}} = \frac{1}{N_0} [F_0^s \delta n + \sigma F_0^a \delta n_s + \frac{1}{k_F^2} F_1^s \vec{k} \cdot \vec{g} + \dots], \quad (107)$$

where  $\delta n = \sum_{k\sigma} \delta n_{k\sigma}$  is the density shift,  $\delta n_s = \sum_{k\sigma} \sigma \delta n_{k\sigma}$  is the spin density shift, and  $\vec{g} = \sum_{k\sigma} \vec{k} \delta n_{k\sigma}$  is the number current. The first two terms can be thought of as molecular field couplings representing the average effect of density and magnetization fluctuations in the surrounding medium on the quasiparticle energy. The third term is the famous “backflow” term which describes the effect of the quasiparticle streaming through the medium to which it couples. The flow pattern is of dipolar form, as depicted in Figure 10. Note that the Landau parameter  $F_1^s$  is not completely independent, as it can be shown that in a Galilean invariant system it is directly related to the effective mass by the relation  $m^*/m = 1 + F_1^s/3$  (see below). In a crystal this relation does not hold.<sup>25</sup>

Before leaving this section, let me just mention that the importance of the *local quasiparticle energy*  $\tilde{\xi}$  or rather the energy *shift*  $\delta\tilde{\xi}$  is

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<sup>24</sup>The structure may remind you of Hartree-Fock theory, to which it is similar, but keep in mind  $f$  is the residual interaction between quasiparticles, not electrons

<sup>25</sup>For an extensive discussion of this and many other aspects of FL theory I’ve glossed over, see G. Baym and C. Pethick, Landau Fermi-Liquid Theory : Concepts and Applications, Wiley 1991

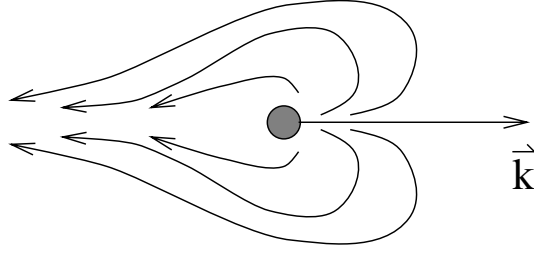


Figure 10: Schematic of backflow around quasiparticle of momentum  $\mathbf{k}$

that when one writes down how external forces couple to the system to determine, e.g. transport properties, it is the gradient of  $\tilde{\xi}_{\mathbf{k}}$  which is the force a qp of momentum  $\mathbf{k}$  experiences due to spatial inhomogeneities in the system. There is a "Landau molecular field" proportional to

$$-\nabla \tilde{\xi}_{\mathbf{k}} = -\nabla \sum_{\mathbf{k}'} f_{\mathbf{k}'\mathbf{k}} \delta n_{\mathbf{k}'}(\mathbf{r}) \quad (108)$$

which is responsible, e.g. for spin waves in dilute gases. Eq. (108) is a simplified version of Landau's famous kinetic equation for a Fermi liquid which is the analog of the Boltzman equation for a weakly interacting gas.

### 2.3.5 Thermodynamic properties

The expression (107) for the quasiparticle energies and the fact that the equilibrium quasiparticle distribution function is just the Fermi function enables immediate calculations of thermodynamic observables in the Fermi liquid. Because the states of the gas and liquid are in one to one correspondence, for example, one immediately knows that the expression

for the entropy of the liquid is the same as that for a free Fermi gas,<sup>26</sup>

$$S = - \sum_{k\sigma} [n_{k\sigma} \log n_{k\sigma} + (1 - n_{k\sigma}) \log(1 - n_{k\sigma})]. \quad (109)$$

Note now that the distribution function  $n_{k\sigma}$  in *local equilibrium* must be a Fermi function evaluated at energy  $\epsilon_{k\sigma}$  given by the bare energy plus the expression (106) in general. However, we are interested in calculating a quantity in *global equilibrium*, in which case the shifts  $\delta n, \delta n_s, \vec{g}, \dots$  vanish. In this case the calculation reduces to the usual one for a free Fermi gas. For temperatures  $T \ll T_F$  we replace the sum  $\sum_{k\sigma}$  by  $N_0 \int d\xi$ . The temperature can then be scaled out, and the remaining integral performed, yielding the entropy density at low temperatures,

$$s = \frac{1}{3} \pi^2 N_0 T, \quad (110)$$

and the specific heat at constant volume is therefore  $C = T(\partial s / \partial T)_V = (m^* k_F / 3) T$ , where in the last step we have used  $N_0 = m^* k_F / \pi^2$ . The result for the liquid is identical to that for the gas, with the exception of the replacement of  $m$  by  $m^*$ .

Similarly, we may derive an expression for the spin susceptibility of the Fermi liquid by constructing the magnetization  $\delta n_s$  as above, and noting that the shift in the distribution function is due to the Landau

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<sup>26</sup>Recall the *form* of the Fermi distribution function for the free gas is obtained purely from combinatorial considerations, not from any knowledge of the energies.

shift in the quasiparticle energy (molecular field) as well as the external field  $\vec{H}$ :

$$\delta n_{k\sigma} = \frac{\partial n_{k\sigma}}{\partial \epsilon_{k\sigma}} (\delta \epsilon_{k\sigma} - \mu_0 \sigma H). \quad (111)$$

Using  $\delta n_s \equiv \sum_{k\sigma} \sigma \delta n_{k\sigma}$ , and noting that since  $\sigma \partial n / \partial \epsilon$  is isotropic and odd in  $\sigma$ , only the  $\ell = 0$ , spin-antisymmetric part of  $\delta \epsilon_{k\sigma}$  contributes to the sum, we find for the spin susceptibility  $\chi_0 = \mu_0 (\partial n_s / \partial H)$

$$\chi = \frac{\mu_0^2 N_0}{(1 + F_0^a)} = \frac{m^*/m}{1 + F_0^a} \chi_0, \quad (112)$$

where  $\chi_0$  is the susceptibility of the free gas.

### 2.3.6 Quasiparticle relaxation time and transport properties.

Calculations of transport properties require introducing the quasiparticle lifetime. Recall the quasiparticle states are *not* eigenstates of the many-body Hamiltonian, due to the weak residual interactions among them. We therefore expect a quasiparticle with momentum  $\vec{k}$  to decay except when it sits exactly at the Fermi surface and when  $T = 0$ , when it can easily be seen there is no phase space for scattering which conserves energy and momentum. But relaxing these conditions ( $\vec{k}$  not on FS,  $T \neq 0$ ) allows phase space for scattering and hence a finite lifetime.

Since the interactions among quasiparticles are assumed weak, we may use a golden rule type formula for the scattering rate”

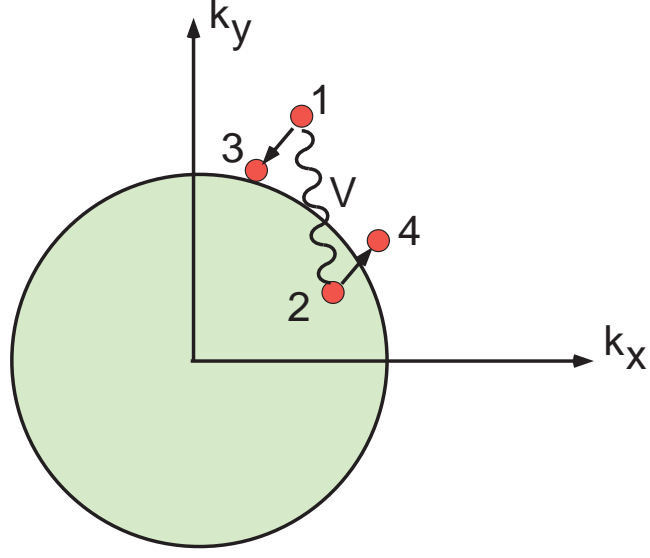


Figure 11: 2-quasiparticle collision: states before (1,2) and after (3,4)

Let's consider a quasiparticle with energy  $\xi_1 = \epsilon_1 - \mu$  above the Fermi level. A scattering process takes it to final state  $\xi_3$ , and to conserve energy and momentum a quasiparticle with energy  $\xi_2$  must be scattered to final state  $\xi_4$ . I've assumed the interaction  $V$  is independent of momentum, frequency, etc. because the most important effects we are looking for are purely statistical, unless  $V$  is very singular.<sup>27</sup> The "golden rule" then gives

$$\begin{aligned} \frac{1}{\tau_1} &= 2\pi \int d\xi_2 N(\xi_2) \int d\xi_3 N(\xi_3) \int d\xi_4 N(\xi_4) |V|^2 f(\xi_2)(1-f(\xi_3))(1-f(\xi_4)) \delta(\xi_1 + \xi_2 - \xi_3 - \xi_4) \simeq \\ &\simeq 2\pi N_0^3 |V|^2 \int_0^{\xi_1} d\xi_3 \int_0^{\xi_1 - \xi_3} d\xi_4 = \pi N_0^3 |V|^2 \xi_1^2, \end{aligned}$$

---

<sup>27</sup>In the case of the Coulomb interaction, which is very singular, screening takes care of this problem. See section 2.2.6

where the delta function conserves energy and the Fermi factors ensure that there is a particle in state 2 and that states 3 and 4 are empty beforehand. For simplicity I evaluated the Fermi functions at  $T=0$ , giving the final simple result. Note I have neglected spin for the moment, but this is not essential.<sup>28</sup> Note now that for  $N_0V \ll 1$  (weak residual interactions) and  $N_0 \sim 1/\varepsilon_F$ , it is clear that for  $\xi \ll \varepsilon_F$  the scattering satisfies the condition

$$\frac{1}{\tau_1} \ll \xi. \quad (113)$$

This means that the quasiparticle states are well-defined near the Fermi surface, since their damping is small compared to the energy of the state. (As expected, the relaxation rate exactly at the Fermi surface vanishes identically.) We therefore expect that Fermi liquid theory calculations in terms of a weakly interacting quasiparticle gas will be valid for frequencies and temperatures such that  $\omega, T \ll \varepsilon_F$ .

Two further comments about the scattering rate are of potential importance. First, I give without proof the full result at finite tempera-

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<sup>28</sup>What I have done which is not really Kosher, however, is to neglect the constraints placed on the scattering by momentum conservation. It turns out in three dimensions this is not terribly important, and one obtains the correct answer. It is a useful exercise to convince yourself, for example, that in 2D the relaxation rate goes like  $\xi^2 \log \xi$ .



tures:<sup>29</sup>

$$\frac{1}{\tau(\xi)} = \frac{\pi|V|^2}{64\varepsilon_F^3}[(\pi T)^2 + \xi^2], \quad (115)$$

so that at finite  $T$  one finds that  $1/\tau$  varies as  $T^2$  or  $\xi^2$ , whichever is larger. Certain simple transport properties in a Fermi liquid reflect this directly. For example, the resistivity due to electron-electron scattering in a metal goes as  $T^2$  at the lowest temperatures; it is usually masked by other, larger sources of scattering in ordinary metals, however.<sup>30</sup> The second remark is that if one were to find, for some microscopic model, that the relaxation rate was larger than the quasiparticle energy, the quasiparticles would be overdamped and the entire concept would be useless. One would then speak of an incoherent or "non-Fermi liquid"

---

<sup>29</sup>Our simple calculation has to be modified to account for momentum conservation, expressed as

$$\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2. \quad (114)$$

Since  $\xi_1$  and  $\xi_2$  are confined to a narrow shell around the Fermi surface, so too are  $\xi_3$  and  $\xi_4$ . This can be seen in Fig. 11, where the requirement that  $\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2$  limits the allowed states for particles 3 and 4. Taking  $\mathbf{k}_1$  fixed, allowed momenta for 2 and 3 are obtained by rotating  $\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2$ ; this rotation is constrained, however, by the fact that particles cannot scatter into occupied states. This restriction on the final states reduces the scattering probability by a factor of  $\xi_1/\varepsilon_F$ , but is the same restriction contained in the calculation above. Thus momentum conservation doesn't affect our  $T = 0$  estimate above, except to modify the prefactor.

If these hand-waving arguments don't satisfy you (they shouldn't), see AGD or Fetter/Wallecka.

<sup>30</sup>Of course this is not quite right. The electron-electron interactions in a solid conserve crystal momentum, and thus the conductivity of a pure crystal would be infinite at any temperature unless one explicitly accounts for Umklapp processes. Thus it is *not* true for the electrical conductivity that  $\sigma \propto \tau$ , with  $\tau$  the 1-particle lifetime due to electron-electron interactions. However the Umklapp processes do also provide a transport rate varying as  $T^2$ , so one often hears the not quite correct remark that the scattering rate in a Fermi liquid varies as  $T^2$ , therefore so does the resistivity  $\rho$ .

system. If, on the other hand, one found that  $1/\tau$  were to scale precisely with  $\max(\xi, T)$  (instead of  $\max(\xi^2, T^2)$ ), the quasiparticles would be in a certain sense critically damped, i.e. not quite well defined, but not completely washed out either. This is what is frequently referred to as a "marginal Fermi liquid".[MFL]

### 2.3.7 Effective mass $m^*$ of quasiparticles

Here I give a quick derivation of the relation between the Landau parameter  $F_{1s}$  which appears in the current and the effective mass  $m^*$ .

The net momentum of the volume  $V$  of quasiparticles is

$$\mathbf{P}_{qp} = 2V \sum_{\mathbf{k}} \mathbf{k} n_{\mathbf{k}}, \text{ net quasiparticle momentum} \quad (116)$$

also the total momentum of the Fermi liquid. Since the number of particles equals the number of quasiparticles, however, the quasiparticle and particle currents must also be equal

$$\mathbf{J}_{qp} = \mathbf{J}_p = 2V \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} n_{\mathbf{k}} \text{ net quasiparticle and particle current} \quad (117)$$

or, since the momentum is just the particle mass times this current

$$\mathbf{P}_p = 2Vm \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} n_{\mathbf{k}} \text{ net quasiparticle and particle momentum} \quad (118)$$

where  $\mathbf{v}_{\mathbf{p}} = \nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}}$ , is the velocity of the quasiparticle. So

$$\sum_{\mathbf{k}} \mathbf{k} n_{\mathbf{k}} = m \sum_{\mathbf{k}} \nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} n_{\mathbf{k}} \quad (119)$$

Let's consider an arbitrary variation of  $n_{\mathbf{k}}$ , and remember that  $\tilde{\epsilon}_{\mathbf{k}}$  depends on  $n_{\mathbf{k}}$ , so that

$$\delta\tilde{\epsilon}_{\mathbf{k}} = 2V \sum_{\mathbf{k}} f_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}'} . \quad (120)$$

For Eq. 119, this means that

$$\begin{aligned} \sum_{\mathbf{k}} \mathbf{k} \delta n_{\mathbf{k}} &= m \sum_{\mathbf{k}} \nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} \delta n_{\mathbf{k}} \\ &\quad + m 2V \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \nabla_{\mathbf{k}} (f_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}'}) n_{\mathbf{k}} , \end{aligned} \quad (121)$$

or integrating by parts (and renaming  $\mathbf{k} \rightarrow \mathbf{k}'$  in the last part), we get

$$\begin{aligned} \sum_{\mathbf{k}} \frac{\mathbf{k}}{m} \delta n_{\mathbf{k}} &= \sum_{\mathbf{k}} \nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} \delta n_{\mathbf{k}} \\ &\quad - 2V \int \sum_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}} f_{\mathbf{k},\mathbf{k}'} \nabla_{\mathbf{k}'} n_{\mathbf{k}'} , \end{aligned} \quad (122)$$

The usual variational argument says that since  $\delta n_{\mathbf{k}}$  is arbitrary, we must have that the integrands are equal

$$\frac{\mathbf{k}}{m} = \nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} - 2V \sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \nabla_{\mathbf{k}'} n_{\mathbf{k}'} \quad (123)$$

At  $T = 0$   $\nabla_{\mathbf{k}'} n_{\mathbf{k}'} = -\hat{k}' \delta(k' - k_F)$ . The integral may now be evaluated by using the system isotropy in  $\mathbf{k}$  space, and choosing  $\mathbf{k}$  parallel  $\hat{z}$ . As we mostly concerned with Fermi surface properties we take  $k = k_F$ , and let  $\theta$  be the angle between  $\mathbf{k}$  (or the z-axis) and  $\mathbf{k}'$ , and finally note that on the Fermi surface  $|\nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}}|_{k=k_F} = v_F = k_F/m^*$ . Thus,

$$\frac{k_F}{m} = \frac{k_F}{m^*} + 2V \int \frac{k'^2 dk d\Omega}{(2\pi\hbar)^3} f_{\mathbf{k},\mathbf{k}'} \hat{k} \cdot \hat{k}' \delta(k' - k_F) \quad (124)$$

However, since both  $\mathbf{k}$  and  $\mathbf{k}'$  are restricted to the Fermi surface  $\hat{k}' = \cos \theta$ , and evaluating the integral over  $k$ , we get

$$\frac{1}{m} = \frac{1}{m^*} + 2V k_F \int \frac{d\Omega}{(2\pi\hbar)^3} f_{\mathbf{k},\mathbf{k}'} \cos \theta, \quad (125)$$

If we now sum over (hidden) spins only the symmetric part of  $f$  appears

$$\frac{1}{m} = \frac{1}{m^*} + \frac{4\pi V k_F}{(2\pi\hbar)^3} \int d(\cos \theta) f^s(\theta) \cos \theta, \quad (126)$$

Now use decomposition (104), orthonormality of Legendre polynomials, and def. of Landau parameters:

$$(127)$$

$$f^\alpha(\theta) = \sum_l f_l^\alpha P_l(\cos \theta), \quad (128)$$

$$\int_{-1}^1 dx P_n(x) P_m(x) dx = \frac{2}{2n+1} \delta_{nm} \quad (129)$$

$$N_0 f_l^\alpha = \frac{V m^* k_F}{\pi^2 \hbar^3} f_l^\alpha = F_l^\alpha, \quad (130)$$

we find that

$$\boxed{\frac{1}{m} = \frac{1}{m^*} + \frac{F_1^s}{3}}, \quad (131)$$

or  $m^*/m = 1 + F_1^s/3$ .

So effective mass and  $F_{1s}$  aren't independent, at least in a Galilean invariant system where (117) holds.

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## Reading:

1. Chs. 31-33, Ashcroft & Mermin
2. Ch. 4, Kittel
3. For a more detailed discussion of the topic, see e.g. D. Mattis, Theory of Magnetism I & II, Springer 1981

## 3 Quantum Magnetism

The main purpose of this section is to introduce you to ordered magnetic states in solids and their “spin wave-like” elementary excitations. Magnetism is an enormous field, and reviewing it entirely is beyond the scope of this course.

### 3.1 Introduction

#### 3.1.1 Atomic magnetic Hamiltonian

The simplest magnetic systems to consider are insulators where electron-electron interactions are weak. If this is the case, the magnetic response of the solid to an applied field is given by the sum of the susceptibilities of the individual atoms. The magnetic susceptibility is defined by the the 2nd derivative of the free energy,<sup>1</sup>

$$\chi = -\frac{\partial^2 F}{\partial H^2}. \quad (1)$$

We would like to know if one can understand (on the basis of an understanding of atomic structure) why some systems (e.g. some

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<sup>1</sup>In this section I choose units such that the system volume  $V = 1$ .

elements which are insulators) are paramagnetic ( $\chi > 0$ ) and some diamagnetic ( $\chi < 0$ ).

The one-body Hamiltonian for the motion of the electrons in the nuclear Coulomb potential in the presence of the field is

$$H_{atom} = \frac{1}{2m} \sum_i \left( \mathbf{p}_i + \frac{e}{c} \mathbf{A}(\mathbf{r}_i) \right)^2 + \sum_i V(r_i) + g_0 \mu_B \mathbf{H} \cdot \mathbf{S}, \quad (2)$$

where  $\sum_i \mathbf{S}_i$  is the total spin operator,  $\mu_B \equiv e/(2mc)$  is the Bohr magneton,  $g_0 \simeq 2$  is the gyromagnetic ratio, and  $\mathbf{A} = -\frac{1}{2} \mathbf{r} \times \mathbf{H}$  is the vector potential corresponding to the applied uniform field, assumed to point in the  $\hat{z}$  direction. Expanding the kinetic energy,  $H_{atom}$  may now be expressed in terms of the orbital magnetic moment operator  $\mathbf{L} = \sum_i \mathbf{r} \times \mathbf{p}_i$  as

$$H_{atom} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i V(r_i) + \delta H, \quad (3)$$

$$\delta H = \mu_B (\mathbf{L} + g_0 \mathbf{S}) \cdot \mathbf{H} + \frac{e^2}{8mc^2} H^2 \sum_i (x_i^2 + y_i^2). \quad (4)$$

Given a set of exact eigenstates for the atomic Hamiltonian in zero field  $|n\rangle$  (ignore degeneracies for simplicity), standard perturbation theory in  $\delta H$  gives

$$\delta E_n = \mathbf{H} \cdot \langle n | \vec{\mu} | n \rangle + \sum_{n' \neq n} \left| \frac{\langle n | \mathbf{H} \cdot \vec{\mu} | n' \rangle}{E_n - E_{n'}} \right|^2 + \frac{e^2}{8mc^2} H^2 \langle n | \sum_i (x_i^2 + y_i^2) | n \rangle, \quad (5)$$

where  $\vec{\mu} = \mu_B (\mathbf{L} + g_0 \mathbf{S})$ . It is easy to see that the first term dominates and is of order the cyclotron frequency  $\omega_c \equiv eH/(mc)$  unless it vanishes for symmetry reasons. The third term is of order  $\omega_c/(e^2/a_0)$  smaller, because typical electron orbits are confined to atomic sizes  $a_0$ , and is important in insulators only when the state  $|n\rangle$  has zero magnetic moment ( $L = S = 0$ ). Since the coefficient

of  $H^2$  is manifestly positive, the susceptibility<sup>2</sup> in the  $\mu = 0$  ground state  $|0\rangle$  is  $\chi = -\partial^2 \delta E_0 / \partial H^2$ , which is clearly  $< 0$ , i.e. diamagnetic.<sup>3</sup>

In most cases, however, the atomic shells are partially filled, and the ground state is determined by minimizing the atomic energy together with the intraatomic Coulomb interaction needed to break certain degeneracies, i.e. by “Hund’s rules”.<sup>4</sup> Once this ground state (in particular the  $S$ ,  $L$ , and  $J$  quantum numbers) is known, the atomic susceptibility can be calculated. The simplest case is again the  $J = 0$  case, where the first term in (5) again vanishes. Then the second term and third term compete, and can result in either a diamagnetic or paramagnetic susceptibility. The 2nd term is called the *Van Vleck* term in the energy. It is paramagnetic since its contribution to  $\chi$  is

$$\chi_{VV} = -\frac{\partial^2 E_0|_{2nd \text{ term}}}{\partial H^2} = 2\mu_B^2 \sum_n \frac{|\langle 0|\vec{\mu}|n'\rangle|^2}{E_n - E_0} > 0. \quad (6)$$

### 3.1.2 Curie Law-free spins

In the more usual case of  $J \neq 0$ , the ground state is  $2J + 1$  degenerate, and we have to be more careful about defining the susceptibility. The free energy as  $T \rightarrow 0$  can no longer be replaced by  $E_0$  as we did above. We have to account for the entropy of the  $2J + 1$  degenerate spin states as well. Applying a magnetic field breaks this degeneracy, so we have a small statistical calculation

---

<sup>2</sup>If the ground state is nondegenerate, we can replace  $F = E - TS$  in the definition of the susceptibility by the ground state energy  $E_0$ .

<sup>3</sup>This weak diamagnetism in insulators with filled shells is called Larmor diamagnetism

<sup>4</sup>See A&M or any serious quantum mechanics book. I’m not going to lecture on this but ask you about it on homework.



to do. The energies of the “spin” in a field are given by

$$H = -\vec{\mu} \cdot \mathbf{H}, \quad (7)$$

and since  $\vec{\mu} = -\gamma \mathbf{J}$  within the subspace of definite  $J^2$ ,<sup>5</sup> the  $2J+1$  degeneracy in  $H = 0$  is completely broken. The free energy is

$$\begin{aligned} F = -T \log Z &= -T \log \sum_{J_z=-J}^J e^{\beta \gamma H J_z} \\ &= -T \log \left[ \frac{e^{\beta \gamma H (J+1/2)} - e^{-\beta \gamma H (J+1/2)}}{e^{\beta \gamma H/2} - e^{-\beta \gamma H/2}} \right], \quad (8) \end{aligned}$$

so the magnetization of the free spins is

$$M = -\frac{\partial F}{\partial H} = \gamma J B(\beta \gamma J H), \quad (9)$$

where  $B(x)$  is the Brillouin function

$$B(x) = \frac{2J+1}{2J} \coth \frac{2J+1}{2J} x - \frac{1}{2J} \coth \frac{1}{2J} x. \quad (10)$$

Note I defined  $\gamma = \mu_B g$ . We were particularly interested in the  $H \rightarrow 0$  case, so as to compare with ions with filled shells or  $J = 0$ ; in this case one expands for  $T \gg \gamma H$ , i.e.  $\coth x \sim 1/x + x/3 + \dots$ ,  $B(x) \simeq (J+1)x/(3J)$  to find the susceptibility

$$\boxed{\chi = -\frac{\partial^2 F}{\partial H^2} = \frac{\gamma^2 J(J+1)}{3T}}, \quad (11)$$

i.e. a *Curie law* for the high-temperature susceptibility. A  $1/T$  susceptibility at high  $T$  is generally taken as evidence for free paramagnetic spins, and the size of the moment given by  $\mu^2 = \gamma^2 J(J+1)$ .

---

<sup>5</sup>This is not obvious at first sight. The magnetic moment *operator*  $\vec{\mu} \propto \hat{\mathbf{L}} + g_0 \hat{\mathbf{S}}$  is not proportional to the total angular momentum *operator*  $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ . However its matrix elements *within the subspace of definite  $L, S, J$*  are proportional, due to the Wigner-Eckart theorem. One therefore may assume the proportionality within the subspace, where the proportionality const.  $\gamma = g(J, L, S) \mu_B$ .  $g$  is called Landé g-factor, and is independent of  $J_z$  according to Wigner-Eckart. See e.g. Ashcroft & Mermin p. 654.

### 3.1.3 Magnetic interactions

The most important interactions between magnetic moments in an insulator are electrostatic and inherently quantum mechanical in nature. From a classical perspective, one might expect two such moments to interact via the classical dipolar force, giving a potential energy of configuration of two moments  $\vec{\mu}_1$  and  $\vec{\mu}_2$  separated by a distance  $\mathbf{r}$  of

$$U = \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \hat{r})(\vec{\mu}_2 \cdot \hat{r})}{r^3} \quad (12)$$

Putting in typical atomic moments of order  $\mu_B = e\hbar/mc$  and distances of order a Bohr radius  $r \sim a_0 = \hbar^2/me^2$ , we find  $U \simeq 10^{-4}eV$ , which is very small compared to typical atomic energies of order  $eV$ . Quantum-mechanical *exchange* is almost always a much larger effect, and the dipolar interactions are therefore normally neglected in the discussions of magnetic interactions in solids. Exchange arises because, e.g., two quantum mechanical spins  $1/2$  (in isolation) can be in either a spin triplet (total  $S = 1$ ), or singlet (total  $S = 0$ ). The spatial part of the two-particle wavefunctions is antisymmetric for triplet and symmetric for singlet, respectively. Since the particles carrying the spins are also charged, there will be a large energetic difference between the two spin configurations due to the different size of the Coulomb matrix elements (the “amount of time the two particles spend close to each other”) in the two cases.<sup>6</sup> In terms of hypothetical atomic wave functions  $\psi_a(\mathbf{r})$  and  $\psi_b(\mathbf{r})$  for the two particles, the singlet and triplet combinations are  $\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)$ , so the singlet-triplet

---

<sup>6</sup>Imagine moving 2 H-atoms together starting from infinite separation. Initially the 3  $S = 1$  states and 1  $S = 0$  states must be degenerate. As the particles start to interact via the Coulomb force at very long range, there will be a splitting between singlet and triplet.

splitting is approximately

$$\begin{aligned} -J \equiv E_0 - E_1 &= \langle 0|H|0\rangle - \langle 1|H|1\rangle \\ &\simeq 2 \int d^3r_1 d^3r_2 \psi_a^*(\mathbf{r}_1) \psi_b^*(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2) \psi_a(\mathbf{r}_2) \psi_b(\mathbf{r}_1) \end{aligned}$$

where  $V$  represents the Coulomb interactions between the particles (and possible other particles in the problem).<sup>7</sup>

We'd now like to write down a simple Hamiltonian for the spins which contains the physics of this exchange splitting. This was done first by Heisenberg (check history here), who suggested

$$H_{2-spin} = J \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \quad (15)$$

You can easily calculate that the energy of the triplet state in this Hamiltonian is  $J/4$ , and that of the singlet state  $-3J/4$ . So the splitting is indeed  $J$ . Note that the sign of  $J$  in the  $H_2$  case is positive, meaning the  $S = 0$  state is favored; the interaction is then said to be antiferromagnetic, meaning it favors antialigning the spins with each other.<sup>8</sup>

The so-called Heitler-London model of exchange just reviewed presented works reasonably well for well-separated molecules, but for  $N$  atoms in a real solid, magnetic interactions are much more complicated, and it is in general not sufficient to restrict one's consideration to the 4-state subspace (singlet  $\oplus$  3 components of

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<sup>7</sup>For example, in the H molecule,

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{e^2}{|\mathbf{R}_1 - \mathbf{R}_2|} - \frac{e^2}{|\mathbf{r}_1 - \mathbf{R}_1|} - \frac{e^2}{|\mathbf{r}_2 - \mathbf{R}_2|}, \quad (14)$$

where  $\mathbf{R}_1$  and  $\mathbf{R}_2$  are the sites of the protons. Note the argument above would suggest naively that the triplet state should be the ground state in the well-separated ion limit, because the Coulomb interaction is minimized in the spatially antisymmetric case. However the true ground state of the  $H_2$  molecule is the Heitler-London *singlet* state  $\psi_s(\mathbf{r}_1, \mathbf{r}_2) \simeq \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)$

<sup>8</sup>Historically the sign convention for  $J$  was the opposite;  $J > 0$  was usually taken to be ferromagnetic, i.e. the Hamiltonian was defined with another minus sign. I use the more popular convention  $H = J \sum S_i \cdot S_j$ . Be careful!

triplet) to calculate the effective exchange. In many cases, particularly when the magnetic ions are reasonably well-separated, it nevertheless turns out to be ok to simply extend the 2-spin form (15) to the entire lattice:

$$H = J \sum_{i\delta} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\delta} \quad (16)$$

where  $J$  is the exchange constant,  $i$  runs over sites and  $\delta$  runs over nearest neighbors.<sup>9</sup> This is the so-called Heisenberg model. The sign of  $J$  can be either antiferromagnetic ( $J > 0$  in this convention), or ferromagnetic ( $J < 0$ ). This may lead, at sufficiently low temperature, to a quantum ordered state with ferromagnetic or antiferromagnetic-type order. Or, it may not. A good deal depends on the type and dimensionality of the lattice, as we discuss below.

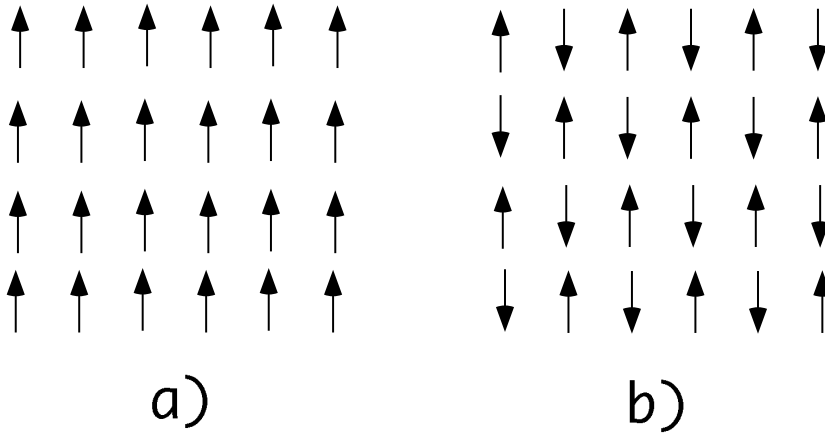


Figure 1: a) Ferromagnetic ordering; b) antiferromagnetic ordering.

Although oversimplified, the Heisenberg model is still very difficult to solve. Fortunately, a good deal has been learned about it, and

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<sup>9</sup>One has to be a bit careful about the counting.  $J$  is defined conventionally such that there is one term in the Hamiltonian for each *bond* between two sites. Therefore if  $i$  runs over all sites, one should have  $\delta$  only run over, e.g. for the simple cubic lattice,  $+\hat{x}$ ,  $+\hat{y}$ , and  $+\hat{z}$ . If it ran over all nearest neighbors, bonds would be double-counted and we would have to multiply by 1/2.

once one has put in the work it turns out to describe magnetic ordering and magnetic correlations rather well for a wide class of solids, provided one is willing to treat  $J$  as a phenomenological parameter to be determined from a fit to experiment.

The simplest thing one can do to take interactions between spins into account is to ask, “What is the average exchange felt by a given spin due to all the other spins?” This is the essence of the *molecular field theory* or *mean field theory* due to Weiss. Split off from the Hamiltonian all terms connecting any spins to a specific spin  $\hat{\mathbf{S}}_i$ . For the nearest-neighbor exchange model we are considering, this means just look at the nearest neighbors. This part of the Hamiltonian is

$$\delta H_i = \hat{\mathbf{S}}_i \cdot \left[ J \sum_{\delta} \hat{\mathbf{S}}_{i+\delta} \right] - \vec{\mu} \cdot \mathbf{H}, \quad (17)$$

where we have included the coupling of the spin in question to the external field as well. We see that the 1-spin Hamiltonian looks like the Hamiltonian for a spin in an effective field,

$$\delta H_i = -\vec{\mu}_i \cdot \mathbf{H}_{eff}, \quad (18)$$

$$\mathbf{H}_{eff} = \mathbf{H} - \frac{J}{g\mu_B} \sum_{\delta} \hat{\mathbf{S}}_{i+\delta} \quad (19)$$

Note this “effective field” as currently defined is a complicated *operator*, depending on the neighboring spin operators  $\hat{\mathbf{S}}_{i+\delta}$ . The mean field theory replaces this quantity with its thermal average

$$\mathbf{H}_{eff} = \mathbf{H} - \frac{J}{g\mu_B} \sum_{\delta} \langle \hat{\mathbf{S}}_{i+\delta} \rangle \quad (20)$$

$$= \mathbf{H} - \frac{zJ}{(g\mu_B)^2} \mathbf{M}, \quad (21)$$

where the magnetization  $M = \langle \mu \rangle$  and  $z$  is the number of nearest neighbors again. But since we have an effective one-body Hamil-

tonian, thermal averages are supposed to be computed just as in the noninteracting system, cf. (9), but in the ensemble with effective magnetic field. Therefore the magnetization is

$$M = \gamma S B(\beta \gamma S H_{eff}) = \gamma S B\left(\beta \gamma S \left[H - \frac{zJ}{\gamma^2} M\right]\right). \quad (22)$$

This is now a nonlinear equation for  $M$ , which we can solve for any  $H$  and  $T$ . It should describe a ferromagnet with finite spontaneous ( $H \rightarrow 0$ ) magnetization below a critical temperature  $T_c$ . So to search for  $T_c$ , set  $H = 0$  and expand  $B(x)$  for small  $x$ :

$$M = -\gamma S B\left(\frac{zJ}{\gamma T_c} M\right) \simeq -\gamma S \frac{S+1}{3S} \frac{zJ}{\gamma T_c} M \quad (23)$$

$$\Rightarrow T_c = \frac{S(S+1)}{3} z(-J), \quad (24)$$

So the critical temperature in this mean field theory (unlike the BCS mean field theory!) is of order the fundamental interaction energy  $|J|$ . We expect this value to be an upper bound to the true critical temperature, which will be suppressed by spin fluctuations about the mean field used in the calculation.

Below  $T_c$ , we can calculate how the magnetization varies near the transition by expanding the Brillouin fctn. to one higher power in  $x$ . The result is

$$M \sim (T - T_c)^{1/2}. \quad (25)$$

Note this exponent  $1/2$  is characteristic of the disappearance of the order parameter near the transition of any mean field theory (Landau).

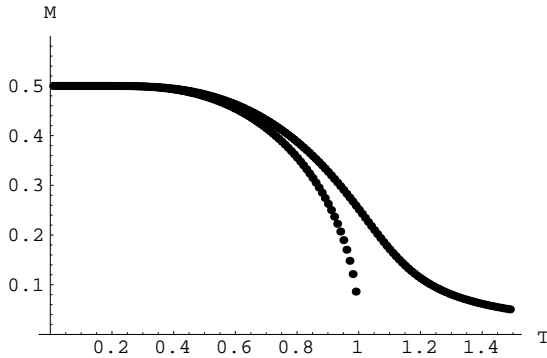


Figure 2: Plot of Mathematica solution to eqn. (22) for  $M$  vs.  $T$  using  $-J = g = 1$ ;  $z = 4$ ;  $S = 1/2$ .  $T_c=1$  for this choice. Upper curve:  $H = 0.1$ ; lower curve:  $H = 0$ .

## 3.2 Ising model

The Ising model<sup>10</sup> consists of a set of spins  $s_i$  with  $z$ -components only localized on lattice sites  $i$  interacting via nearest-neighbor exchange  $J < 0$ :

$$\mathcal{H} = J \sum_{i,j \in n.n.} S_i S_j - 2\mu_B H \sum_i S_i. \quad (26)$$

Note it is an inherently *classical* model, since all spin commutators vanish  $[S_i, S_j] = 0$ . Its historical importance consisted not so much in its applicability to real ferromagnetic systems as in the role its solutions, particularly the analytical solution of the 2D model published by Onsager in 1944, played in elucidating the nature of phase transitions. Onsager's solution demonstrated clearly that all approximation methods and series expansions heretofore used to attack the ferromagnetic transition failed in the critical regime, and thereby highlighted the fundamental nature of the problem of critical phenomena, not solved (by Wilson and others) until in the early 70's.

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<sup>10</sup>The "Ising model" was developed as a model for ferromagnetism by Wilhelm Lenz and his student Ernst Ising in the early '20's.

### 3.2.1 Phase transition/critical point

We will be interested in properties of the model (26) at low and at high temperatures. What we will find is that there is a temperature  $T_c$  below which the system magnetizes spontaneously, just as in mean field theory, but that its true value is in general smaller than that given by mean field theory due to the importance of thermal fluctuations. Qualitatively, the phase diagram looks like this:

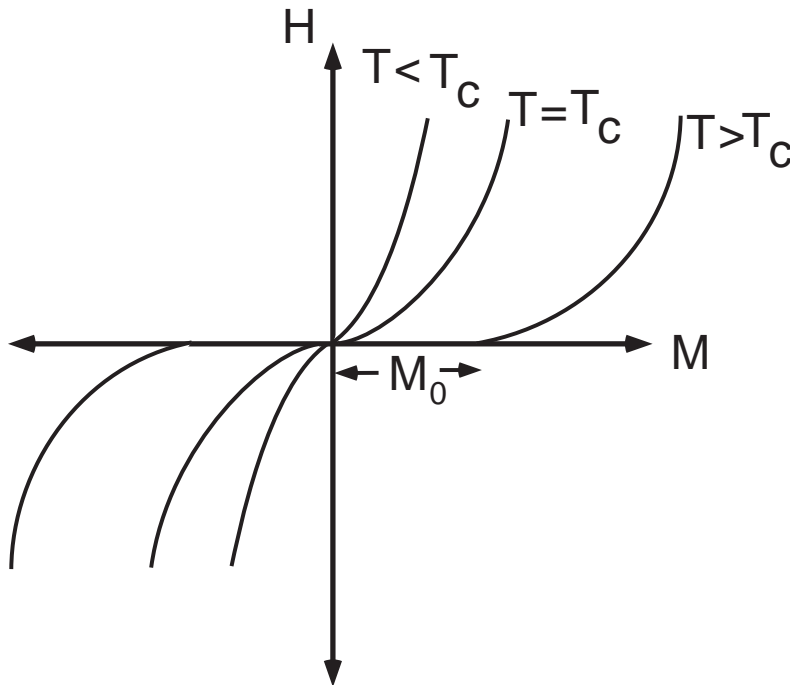


Figure 3: Field-magnetization curves for three cases.  $M_0$  is spontaneous magnetization in ferromagnetic phase  $T < T_c$ .

Below  $T_c$ , the system magnetizes spontaneously even for field  $H \rightarrow 0$ . Instead of investigating the Onsager solution in detail, I will rely on the Monte Carlo simulation of the model developed by Jim Sethna and Bob Silsbee as part of the Solid State Simulation (SSS) project. The idea is as follows. We would like to minimize  $F = T \log \text{Tr} \exp -\beta H$  for a given temperature and ap-



plied field. Finding the configuration of Ising spins which does so is a complicated task, but we can imagine starting the system at high temperatures, where all configurations are equally likely, and cooling to the desired temperature  $T$ .<sup>11</sup> Along the way, we allow the system to relax by “sweeping” through all spins in the finite size lattice, and deciding in the next Monte Carlo “time” step whether the spin will be up or down. Up and down are weighted by a Boltzman probability factor

$$p(S_i = \pm 1/2) = \frac{e^{\pm \mu H_{eff}/T}}{e^{-\mu H_{eff}/T} + e^{\mu H_{eff}/T}}, \quad (27)$$

where  $H_i^{eff}$  is the effective field defined in (19). The simulation picks a spin  $S_i$  in the next time step randomly, but weighted with these up and down probabilities. A single “sweep” (time step) consists of  $L \times L$  such attempts to flip spins, where  $L$  is the size of the square sample. Periodic boundary conditions are assumed, and the spin configuration is displayed, with one color for up and one for down.

Here are some remarks on Ising critical phenomena, some of which you can check yourself with the simulation:

- At high temperatures one recovers the expected Curie law  $\chi \sim 1/T$
- The susceptibility diverges at a critical temperature below the mean field value.<sup>12</sup> Near, but not too near, the transition  $\chi$  has the Curie-Weiss form  $\chi \sim (T - T_c)^{-1}$ .
- With very careful application of the simulation, one should obtain Onsager’s result that very near the transition (“critical

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<sup>11</sup>This procedure is called simulated annealing

<sup>12</sup>This is given as a homework problem. Note the value of  $J$  used in the simulation is  $1/4$  that defined here, since  $S$ ’s are  $\pm 1$ .

regime”)

$$M \sim (T_c - T)^\beta, \quad (28)$$

with  $\beta = 1/8$ . The susceptibility actually varies as

$$\chi \sim |T - T_c|^{-\gamma}, \quad (29)$$

with  $\gamma = 7/4$ . Other physical quantities also diverge near the transition, e.g. the specific heat varies as  $|T - T_c|^{-\alpha}$ , with  $\alpha = 0$  (log divergence).

- There is no real singularity in any physical quantity so long as the system size remains finite.
- The critical exponents  $\alpha, \beta, \gamma \dots$  get closer to their mean field values ( $\beta = 1/2, \alpha = 0, \gamma = 7/4, \dots$ ) as the number of nearest neighbors in the lattice increases, or if the dimensionality of the system increases.
- The mean square size of thermal magnetization fluctuations gets very large close to the transition (“Critical opalescence”, so named for the increased scattering of light near the liquid-solid critical point).
- Magnetization relaxation gets very long near the transition (“Critical slowing down”).
- In 1D there is no finite temperature phase transition, although mean field theory predicts one. See next section.

### 3.2.2 1D solution by transfer matrix

### 3.2.3 Ferromagnetic domains

## 3.3 Ferromagnetic magnons

Let's consider the simplest example of an insulating ferromagnet, described by the ferromagnetic Heisenberg Hamiltonian

$$H = J \sum_{i\delta} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\delta} - 2\mu_B H_0 \sum_i \hat{S}_{iz}, \quad (30)$$

where  $J < 0$  is the ferromagnetic exchange constant,  $i$  runs over sites and  $\delta$  runs over nearest neighbors, and  $H_0$  is the magnetic field pointing in the  $\hat{z}$  direction. It is clear that the system can minimize its energy by having all the spins  $\mathbf{S}$  align along the  $\hat{z}$  direction at  $T = 0$ ; i.e. the quantum ground state is identical to the classical ground state. Finding the elementary excitations of the quantum many-body system is not so easy, however, due to the fact that the spin operators do not commute.

### 3.3.1 Holstein-Primakoff transformation

One can attempt to transform the spin problem to a more standard many-body interacting problem by replacing the spins with boson creation and annihilation operators. This can be done *exactly* by the Holstein-Primakoff transformation<sup>13</sup>

$$\hat{S}_i^+ = \hat{S}_{ix} + i\hat{S}_{iy} = (2S)^{1/2} \left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2} a_i \quad (31)$$

$$\hat{S}_i^- = \hat{S}_{ix} - i\hat{S}_{iy} = (2S)^{1/2} a_i^\dagger \left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2}. \quad (32)$$

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<sup>13</sup>T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).

Verify for yourselves that these definitions  $S_i^\pm$  give the correct commutation relations  $[\hat{S}_x, \hat{S}_y] = i\hat{S}_z$  if the bosonic commutation relations  $[a, a^\dagger] = 1$  are obeyed on a given lattice site. Note also that the operators which commute with the Hamiltonian are  $\hat{S}^2$  and  $\hat{S}_z$  as usual, so we can classify all states in terms of their eigenvalues  $S(S+1)$  and  $S_z$ . To complete the algebra we need a representation for  $\hat{S}_z$ , which can be obtained by using the identity (on a given site  $i$ )

$$\hat{S}_z^2 = S(S+1) - \frac{1}{2}(\hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+). \quad (33)$$

Using (32) and some tedious applications of the bosonic commutation relations, we find

$$\hat{S}_z = S - a^\dagger a. \quad (34)$$

Now since the system is periodic, we are looking for excitations which can be characterized by a well-defined momentum (crystal momentum)  $\mathbf{k}$ , so we define the Fourier transformed variables

$$a_i = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{x}_i} b_{\mathbf{k}} \quad ; \quad a_i^\dagger = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}_i} b_{\mathbf{k}}^\dagger, \quad (35)$$

where as usual the F.T. variables also satisfy the bosonic relations  $[b_{\mathbf{k}}, b_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}$ , etc. Looking forward a bit, we will see that the operators  $b_{\mathbf{k}}^\dagger$  and  $b_{\mathbf{k}}$  create and destroy a *magnon* or *spin-wave* excitation of the ferromagnet. These turn out to be excitations where the spins locally deviate only a small amount from their ground state values ( $\parallel \hat{z}$ ) as the “spin wave” passes by. This suggests *a posteriori* that an expansion in the spin *deviations*  $a_i^\dagger a_i$  (see (34)) may converge quickly. Holstein and Primakoff therefore suggested expanding the nasty square roots in (32), giving

$$\begin{aligned}
\hat{S}_i^+ &\simeq (2S)^{1/2} \left[ a_i - \left( \frac{a_i^\dagger a_i a_i}{4S} \right) + \dots \right] \\
&= \left( \frac{2S}{N} \right)^{1/2} \left[ \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_i} b_{\mathbf{k}} - \frac{1}{4SN} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{k}''} e^{i(\mathbf{k} - \mathbf{k}' - \mathbf{k}'') \cdot \mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}''} + \dots \right] \quad (36)
\end{aligned}$$

$$\begin{aligned}
\hat{S}_i^- &\simeq (2S)^{1/2} \left[ a_i^\dagger - \left( \frac{a_i^\dagger a_i^\dagger a_i}{4S} \right) + \dots \right] \\
&= \left( \frac{2S}{N} \right)^{1/2} \left[ \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_i} b_{\mathbf{k}}^\dagger - \frac{1}{4SN} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{k}''} e^{i(\mathbf{k} + \mathbf{k}' - \mathbf{k}'') \cdot \mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'}^\dagger b_{\mathbf{k}''} + \dots \right] \quad (37)
\end{aligned}$$

$$\hat{S}_{iz} = S - a_i^\dagger a_i = S - \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'}. \quad (38)$$

Note that the expansion is formally an expansion in  $1/S$ , so we might expect it to converge rapidly in the case of a large-spin system.<sup>14</sup> The last equation is exact, not approximate, and it is useful to note that the total spin of the system along the magnetic field is

$$S_{z,tot} = \sum_i S_z = NS - \frac{1}{N} \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \quad (39)$$

consistent with our picture of magnons tipping the spin away from its  $T = 0$  equilibrium direction along the applied field.

### 3.3.2 Linear spin wave theory

The idea now is to keep initially only the bilinear terms in the magnon operators, leaving us with a soluble Hamiltonian, hoping that we can then treat the 4th-order and higher terms pertur-

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<sup>14</sup>For spin-1/2, the case of greatest interest, however, it is far from obvious that this uncontrolled approximation makes any sense, despite the words we have said about spin deviations being small. Why should they be? Yet empirically linear spin wave theory works very well in 3D, and surprisingly well in 2D.

batively.<sup>15</sup> Simply substitute (36)-(38) into (30), and collect the terms first proportional to  $S^2$ ,  $S$ , 1,  $1/S$ , etc. We find

$$H = \frac{1}{2}JNzS^2 - 2\mu_B H_0 S + H_0^{magnon} + \mathcal{O}(1), \quad (40)$$

where  $z$  is the number of nearest neighbors (e.g. 6 for simple cubic lattice), and

$$\begin{aligned} H_0^{magnon} &= \frac{JS}{N} \sum_{i\delta\mathbf{k}\mathbf{k}'} \left[ e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} e^{i\mathbf{k}'\cdot\delta} b_{\mathbf{k}} b_{\mathbf{k}}^\dagger + e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} e^{-i\mathbf{k}'\cdot\delta} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \right. \\ &\quad \left. - e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} - e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{R}_i+\delta)} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \right] + \frac{2\mu_B H_0}{N} \sum_{i\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \\ &= JzS \sum_{\mathbf{k}} \left[ \gamma_{\mathbf{k}} b_{\mathbf{k}} b_{\mathbf{k}}^\dagger + \gamma_{-\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - 2b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \right] + 2\mu_B H_0 \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} [-2JzS(1 - \gamma_{\mathbf{k}}) + 2\mu_B H_0] b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \end{aligned} \quad (41)$$

where

$$\gamma_k = \frac{1}{z} \sum_{\delta} e^{i\mathbf{k}\cdot\delta} \quad (42)$$

is the magnon dispersion function, which in this approximation depends only on the positions of the nearest neighbor spins. Note in the last step of (41), I assumed  $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}$ , which is true for lattices with inversion symmetry. For example, for the simple cubic lattice in 3D with lattice constant  $a$ ,  $\gamma_{\mathbf{k}} = (\cos k_x a + \cos k_y a + \cos k_z a)/3$ , clearly an even function of  $\mathbf{k}$ . Under these assumptions, the magnon part of the Hamiltonian is remarkably simple, and can be written like a harmonic oscillator or phonon-type Hamiltonian,  $H_0^{magnon} = \sum_{\mathbf{k}} n_{\mathbf{k}} \omega_{\mathbf{k}}$ , where  $n_{\mathbf{k}} = b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$  is the number of magnons in state  $\mathbf{k}$ , and

$$\omega_k = -JSz(1 - \gamma_{\mathbf{k}}) + 2\mu_B H_0 \quad (43)$$

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<sup>15</sup>physically these “nonlinear spin wave” terms represent the interactions of magnons, and resemble closely terms representing interactions of phonons in anharmonic lattice theory

is the magnon dispersion. The most important magnons will be those with momenta close to the center of the Brillouin zone,  $k \sim 0$ , so we need to examine the small- $k$  dispersion function. For a Bravais lattice, like simple cubic, this expansion gives  $1 - \gamma_{\mathbf{k}} \simeq k^2$ ,<sup>16</sup> i.e. the magnon dispersion vanishes as  $k \rightarrow 0$ . For more complicated lattices, there will be solutions with  $\omega_{\mathbf{k}} \rightarrow \text{const.}$  There is always a “gapless mode”  $\omega_{\mathbf{k}} \rightarrow 0$  as well, however, since the existence of such a mode is guaranteed by the Goldstone theorem.<sup>17</sup> The figure shows a simple 1D schematic of a spin wave

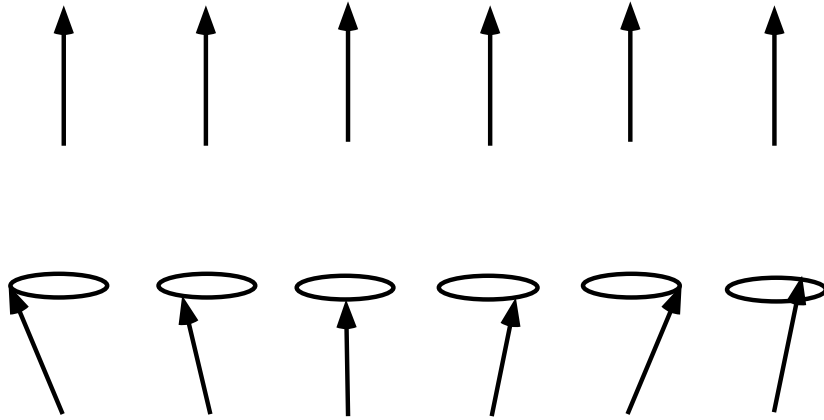


Figure 4: Real space picture of spin deviations in magnon. Top: ordered ground state

with wavelength  $\lambda = 2\pi/k$  corresponding to about 10 lattice sites. The picture is supposed to convey the fact that the spin deviations from the ordered state are small, and vary slightly from site to site. Quantum mechanically, the wave function for the spin wave state contains at each site a small amplitude for the spin to be in a state with definite  $S_x$  and/or  $S_y$ . This can be seen by inverting Eq. (37) to leading order, & noting that the spin wave creation operator  $b_{\mathbf{k}}^\dagger$  lowers the spin with  $\hat{\mathbf{S}}^- = \hat{S}_x - i\hat{S}_y$  with phase  $e^{-i\mathbf{k}\cdot\mathbf{R}_i}$  and amplitude  $\sim 1/S$  at each site  $i$ .

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<sup>16</sup>Check for simple cubic!

<sup>17</sup>For every spontaneously broken continuous symmetry of the Hamiltonian there is a  $\omega_{\mathbf{k}\rightarrow 0} = 0$  mode.

### 3.3.3 Dynamical Susceptibility

#### Experimental interlude

The simple spin wave calculations described above (and below) are uncontrolled for spin-1/2 systems, and it would be nice to know to what extent one can trust them. In recent years, numerical work (exact diagonalization and quantum Monte Carlo) techniques have shown, as noted, that linear spin wave calculations compare surprisingly well with such “exact” results for the Heisenberg model. But we still need to know if there are any physical systems whose effective spin Hamiltonian can really be described by Heisenberg models. In addition, keep in mind that the utility of spin wave theory was recognized long before such numerical calculations were available, mainly through comparison with experiments on simple magnets. The most useful probe of magnetic structure is slow neutron scattering, a technique developed in the 40’s by Brockhouse and Schull (Nobel prize 1994). This section is a brief discussion of how one can use neutron scattering techniques to determine the dispersion and lifetimes of magnetic excitations in solids.<sup>18</sup>

Neutrons scatter from solids primarily due to the nuclear strong force, which leads to nonmagnetic neutron-ion scattering and allows structural determinations very similar to x-ray diffraction analysis. In addition, slow neutrons traversing a crystal can emit or absorb phonons, so the inelastic neutron cross-section is also a sensitive measure of the dispersion of the collective modes of the ionic system.<sup>19</sup> There is also a force on the neutron due to

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<sup>18</sup>A complete discussion is found in Lovesey, *Theory of Neutron Scattering from Condensed Matter*, Oxford 1984, V. 2

<sup>19</sup>cf. Ashcroft & Mermin ch. 24



the interaction of its small magnetic dipole moment with the spin magnetic moment of the electrons in the solid. There are therefore additional contributions to the peaks in the elastic neutron scattering intensity (at the Bragg angles) corresponding to magnetic scattering if the solid has long-range magnetic order; they can be distinguished from the nonmagnetic scattering because the additional spectral weight is strongly temperature dependent and disappears above the critical temperature, or through application of an external magnetic field. Furthermore, in analogy to the phonon case, inelastic neutron scattering experiments on ferromagnets yield peaks corresponding to processes where the neutron absorbs or emits a spin wave excitation. Thus the dispersion relation for the magnons can be mapped out.<sup>20</sup>

I will not go through the derivation of the inelastic scattering cross section, which can be found in Lovesey's book. It is similar to the elementary derivation given by Ashcroft & Mermin in Appendix N for phonons. The result is

$$\begin{aligned} \left( \frac{d^2\sigma}{d\Omega d\omega} \right)_{inel} &= a_0^2 \frac{k'}{k} \left\{ \frac{g}{2} F(\mathbf{q}) \right\}^2 e^{-2W(\mathbf{q})} (1 + b(\omega)) \\ &\times \frac{-N}{\pi(g\mu_B)^2} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) \text{Im } \chi_{\alpha\beta}(\mathbf{q}, -\omega) \end{aligned} \quad (44)$$

where  $a_0$  is the Bohr radius,  $\mathbf{k}$  and  $\mathbf{k}'$  are initial and final wave vector,  $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ ,  $F(\mathbf{q})$  atomic form factor,  $e^{-2W(\mathbf{q})}$  the Debye-Waller factor, and  $b(\omega)$  the Bose distribution function,  $N$  the number of unit cells, and  $\omega$  is the energy change of the neutron,

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<sup>20</sup>Even in systems without long range magnetic order, neutron experiments provide important information on the correlation length and lifetime of *spin fluctuations*. In strongly correlated systems (e.g. magnets just above their critical temperature, or itinerant magnets close to a magnetic transition as in Sec. xxx), these can be thought of as collective modes with finite lifetime and decay length. This means the correlation function  $\langle \hat{\mathbf{S}}_i^\alpha(t) \hat{\mathbf{S}}_j^\alpha \rangle$  is not const. as  $t, |\mathbf{R}_i - \mathbf{R}_j| \rightarrow \infty$ , but may fall off very slowly, as “power laws”  $t^{-\beta}$ ,  $|\mathbf{R}_i - \mathbf{R}_j|^{-\gamma}$ .

$k^2/(2m) - k'^2/(2m)$ . The physics we are interested in is contained in the imaginary part of the dynamic susceptibility  $\chi(\mathbf{q}, \omega)$ . For  $\omega < 0$ , this measures the energy loss by neutrons as they slow down while emitting spin waves in the solid; for  $\omega > 0$  the neutrons are picking up energy from thermally excited spin waves.

By spin rotational invariance, all components  $\chi_{zz} = \chi_{xx} = \chi_{yy}$  are equal. It is then most convenient to calculate—within linear spin wave theory—the transverse spin susceptibility

$$\chi_{+-}^R(\mathbf{R}_i - \mathbf{R}_j, t) \equiv -\text{Tr} \left( \hat{\rho} [\hat{\mathbf{S}}_i^+(t), \hat{\mathbf{S}}_j^-] \right) \theta(t) \quad (45)$$

and then its Fourier transform wrt momentum  $\mathbf{q}$  and frequency  $\omega$ . I won't do this calculation explicitly, but leave it as an exercise. Note it follows exactly the method used to calculate the charge susceptibility on p. 22 of the previous section. You express the  $S$  operators in terms of the  $b_k$ 's, whose time dependence is exactly known since the approximate Hamiltonian is quadratic. At the end, after Fourier transforming, one recovers

$$\chi_{+-}(\mathbf{q}, \omega) = \left( \frac{2S}{N} \right) \left( \frac{1}{\omega + \omega_{\mathbf{q}} + i0^+} \right). \quad (46)$$

Again, as for the Fermi gas, we see that the collective modes of the system are reflected as the poles in the appropriate response function.

The final cross section is now proportional to

$$\text{Im } \chi_{+-}(\mathbf{q}, -\omega) \sim \delta(\omega + \omega_{\mathbf{q}}), \quad (47)$$

i.e. there is a peak when a magnon is *absorbed* (neutron's energy  $k'^2/(2m)$  is larger than initial energy  $k^2/(2m) \Rightarrow \omega \equiv k^2/(2m) - k'^2/(2m) < 0$ ). There is another similar contribution

proportional to  $\delta(\omega - \omega_{\mathbf{q}})$  (emission) coming from  $\chi_{-+}$ . Thus the dispersion  $\omega_{\mathbf{q}}$  can be mapped out by careful measurement.

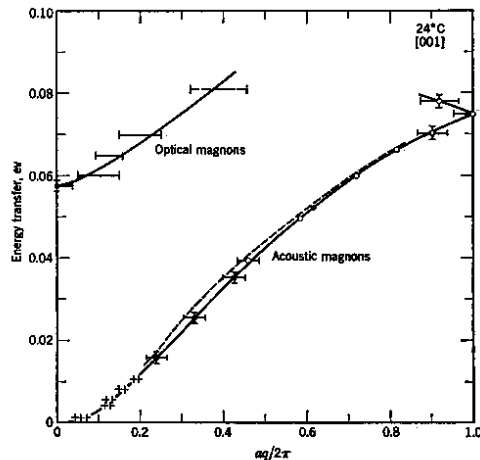


Figure 5: Neutron scattering data on ferromagnet. I searched a bit but couldn't come up with any more modern data than this. This is Fig. 1, Ch. 4 of Kittel, Magnon dispersions in magnetite from inelastic neutron scattering by Brockhouse (Nobel Prize 1994) and Watanabe.

The one-magnon lines are of course broadened by magnon-magnon interactions, and by finite temperatures (Debye-Waller factor). There are also multimagnon absorption and emission processes which contribute in higher order.

### 3.4 Quantum antiferromagnet

Antiferromagnetic systems are generally approached by analogy with ferromagnetic systems, assuming that the system can be divided up into two or more *sublattices*, i.e. infinite interpenetrating subsets of the lattice whose union is the entire lattice. Classically, it is frequently clear that if we choose all spins on a given judiciously chosen sublattice to be aligned with one another, we must achieve a minimum in the energy. For example, for the classical

AF Heisenberg model  $H = J \sum_{i\delta} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta}$  with  $J > 0$  on a square lattice, choosing the A-B sublattices in the figure and making all spins up on one and down on another allows each bond to achieve its lowest energy of  $-JS^2$ . This state, with alternating up and down spins, is referred to as the classical Néel state. Similarly, it may be clear to you that on the triangular lattice the classical lowest energy configuration is achieved when spins are placed at  $120^\circ$  with respect to one another on the sublattices  $A, B, C$ . However,

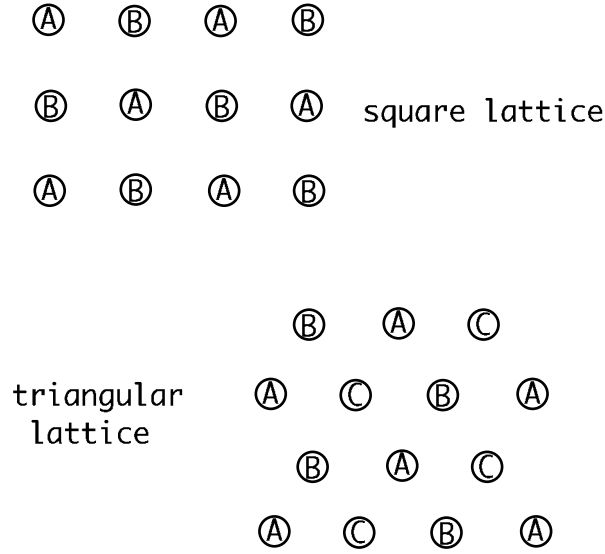


Figure 6: Possible choice of sublattices for antiferromagnet

quantum magnetic systems are not quite so simple. Consider the magnetization  $M_A$  on a given sublattice (say the A sites in the figure) of the square lattice; alternatively one can define the *staggered magnetization* as  $M_s = \sum_i (-1)^i \langle \hat{\mathbf{S}}_i \rangle$  (Note  $(-1)^i$  means  $+1$  on the A sites and  $-1$  on the B sites.) Either construct can be used as the order parameter for an antiferromagnet on a bipartite lattice. In the classical Néel state, these are simply  $M_A = NS/2$  and  $M_s = NS$ , respectively, i.e. the sublattice or staggered magnetization are saturated. In the wave function for the ground

state of a *quantum* Heisenberg antiferromagnet, however, there is some amplitude for spins to be flipped on a given sublattice, due to the fact that for a given bond the system can lower its energy by taking advantage of the  $\hat{S}_x\hat{S}'_x + \hat{S}_y\hat{S}'_y$  terms. This effect can be seen already by examining the two-spin 1/2 case for the ferromagnet and antiferromagnet. For the ferromagnet, the classical energy is  $-|J|S^2 = -|J|/4$ , but the quantum energy in the total spin 1 state is also  $-|J|/4$ . For the antiferromagnet, the classical energy is  $-JS^2 = -J/4$ , but the energy in the total spin 0 quantum mechanical state is  $-3J/4$ . So quantum fluctuations—which inevitably depress the magnetization on a given sublattice—lower the energy in the antiferromagnetic case. This can be illustrated in a very simple calculation of magnons in the antiferromagnet following our previous discussion in section 7.2.

### 3.4.1 Antiferromagnetic magnons

We will follow the same procedure for the ferromagnet on each sublattice A and B, defining

$$\hat{S}_i^{A+} = \hat{S}_{ix}^A + i\hat{S}_{iy}^A = (2S)^{1/2} \left(1 - \frac{A_i^\dagger A_i}{2S}\right)^{1/2} A_i \quad (48)$$

$$\hat{S}_i^{A-} = \hat{S}_{ix}^A - i\hat{S}_{iy}^A = (2S)^{1/2} A_i^\dagger \left(1 - \frac{A_i^\dagger A_i}{2S}\right)^{1/2} \quad (49)$$

$$\hat{S}_i^{B+} = \hat{S}_{ix}^B + i\hat{S}_{iy}^B = (2S)^{1/2} \left(1 - \frac{B_i^\dagger B_i}{2S}\right)^{1/2} B_i \quad (50)$$

$$\hat{S}_i^{B-} = \hat{S}_{ix}^B - i\hat{S}_{iy}^B = (2S)^{1/2} B_i^\dagger \left(1 - \frac{B_i^\dagger B_i}{2S}\right)^{1/2} \quad (51)$$

$$S_{iz}^A = S - A_i^\dagger A_i \quad (52)$$

$$-S_{iz}^B = S - B_i^\dagger B_i, \quad (53)$$

i.e. we assume that in the absence of any quantum fluctuations spins on sublattice A are up and those on B are down. Otherwise the formalism on each sublattice is identical to what we did for the ferromagnet. We introduce on each sublattice creation & annihilation operators for spin waves with momentum  $\mathbf{k}$ :

$$a_{\mathbf{k}} = \frac{1}{N^{1/2}} \sum_{i \in A} A_i e^{i\mathbf{k} \cdot \mathbf{R}_i}; \quad a_{\mathbf{k}}^\dagger = \frac{1}{N^{1/2}} \sum_{i \in A} A_i^\dagger e^{-i\mathbf{k} \cdot \mathbf{R}_i} \quad (54)$$

$$b_{\mathbf{k}} = \frac{1}{N^{1/2}} \sum_{i \in B} B_i e^{i\mathbf{k} \cdot \mathbf{R}_i}; \quad b_{\mathbf{k}}^\dagger = \frac{1}{N^{1/2}} \sum_{i \in B} B_i^\dagger e^{-i\mathbf{k} \cdot \mathbf{R}_i}. \quad (55)$$

In principle  $\mathbf{k}$  takes values only in the 1st *magnetic Brillouin zone*, or *half-zone*, since the periodicity of the sublattices is twice that of the underlying lattice. The spin operators on a given site are then expanded as

$$\hat{S}_i^{A+} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[ \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_i} a_{\mathbf{k}} + \dots \right], \quad (56)$$

$$\hat{S}_i^{B+} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[ \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_i} b_{\mathbf{k}} + \dots \right], \quad (57)$$

$$\hat{S}_i^{A-} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[ \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_i} a_{\mathbf{k}}^\dagger + \dots \right], \quad (58)$$

$$\hat{S}_i^{B-} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[ \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_i} b_{\mathbf{k}}^\dagger + \dots \right], \quad (59)$$

$$\hat{S}_{iz}^A = S - \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \quad (60)$$

$$\hat{S}_{iz}^B = -S + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}. \quad (61)$$

The expansion of the Heisenberg Hamiltonian in terms of these variables is now (compare (40))

$$H = -NzJS^2 + H_0^{magnon} + \mathcal{O}(1), \quad (62)$$

$$H_0^{magnon} = JzS \sum_{\mathbf{k}} \left[ \gamma_{\mathbf{k}} (A_{\mathbf{k}}^\dagger B_{\mathbf{k}}^\dagger + A_{\mathbf{k}} B_{\mathbf{k}}) + (A_{\mathbf{k}}^\dagger A_{\mathbf{k}} + B_{\mathbf{k}}^\dagger B_{\mathbf{k}}) \right] \quad (63)$$

Unlike the ferromagnetic case, merely expressing the Hamiltonian to bilinear order in the magnon variables does not diagonalize it immediately. We can however perform a canonical transformation<sup>21</sup> to bring the Hamiltonian into diagonal form (check!):

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} A_{\mathbf{k}} - v_{\mathbf{k}} B_{\mathbf{k}}^\dagger; \quad \alpha_{\mathbf{k}}^\dagger = u_{\mathbf{k}} A_{\mathbf{k}}^\dagger - v_{\mathbf{k}} B_{\mathbf{k}} \quad (64)$$

$$\beta_{\mathbf{k}} = u_{\mathbf{k}} B_{\mathbf{k}} - v_{\mathbf{k}} A_{\mathbf{k}}^\dagger; \quad \beta_{\mathbf{k}}^\dagger = u_{\mathbf{k}} B_{\mathbf{k}}^\dagger - v_{\mathbf{k}} A_{\mathbf{k}}, \quad (65)$$

where the coefficients  $u_{\mathbf{k}}, v_{\mathbf{k}}$  must be chosen such that  $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ . One such choice is  $u_{\mathbf{k}} = \cosh \theta_{\mathbf{k}}$  and  $v_{\mathbf{k}} = \sinh \theta_{\mathbf{k}}$ . For each  $\mathbf{k}$ , choose the angle  $\theta_{\mathbf{k}}$  such that the anomalous terms like  $A_{\mathbf{k}}^\dagger B_{\mathbf{k}}^\dagger$  vanish. One then finds the solution

$$\tanh 2\theta_{\mathbf{k}} = -\gamma_{\mathbf{k}}, \quad (66)$$

and

$$H_0^{magnon} = -NE_J + \sum_{\mathbf{k}} \omega_{\mathbf{k}} (\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} + 1), \quad (67)$$

where

$$\omega_{\mathbf{k}}^2 = E_J^2 (1 - \gamma_{\mathbf{k}}^2), \quad (68)$$

and  $E_J = JzS$ . Whereas in the ferromagnetic case we had  $\omega_{\mathbf{k}} \sim (1 - \gamma_{\mathbf{k}}) \sim k^2$ , it is noteworthy that in the antiferromagnetic case

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<sup>21</sup>The definition of a canonical transformation, I remind you, is one which will give canonical commutation relations for the transformed fields. This is important because it ensures that we can interpret the Hamiltonian represented in terms of the new fields as a (now diagonal) fermion Hamiltonian, read off the energies, etc.

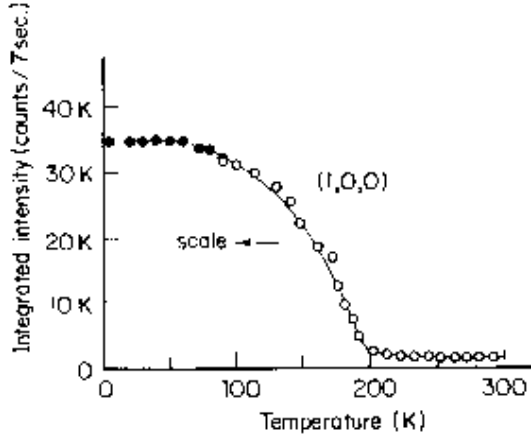


Figure 7: Integrated intensity of (100) Bragg peak vs. temperature for  $\text{LaCuO}_4$ , with  $T_N = 195\text{K}$ . (After Shirane et al. 1987)

the result  $\omega_{\mathbf{k}} \sim (1 - \gamma_{\mathbf{k}})^{1/2} \sim k$  gives a linear magnon dispersion at long wavelengths (a center of symmetry of the crystal must be assumed to draw this conclusion). Note further that for each  $\mathbf{k}$  there are two degenerate modes in  $H_0^{\text{magnon}}$ .

### 3.4.2 Quantum fluctuations in the ground state

At  $T = 0$ , there are no thermally excited spin wave excitations. Nevertheless the spin wave theory yields an decrease of the ground state energy relative to the classical value  $-NJzS^2$ , but an *increase* over the quantum ferromagnet result of  $-N|J|S(S+1)$  due to the zero-point (constant) term in (67).<sup>22</sup> The ground-state energy is

$$E_0 \simeq -NE_J + \sum_{\mathbf{k}} \omega_{\mathbf{k}}. \quad (69)$$

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<sup>22</sup>Recall the classical Néel state, which does not contain such fluctuations, is *not* an eigenstate of the quantum Heisenberg Hamiltonian.



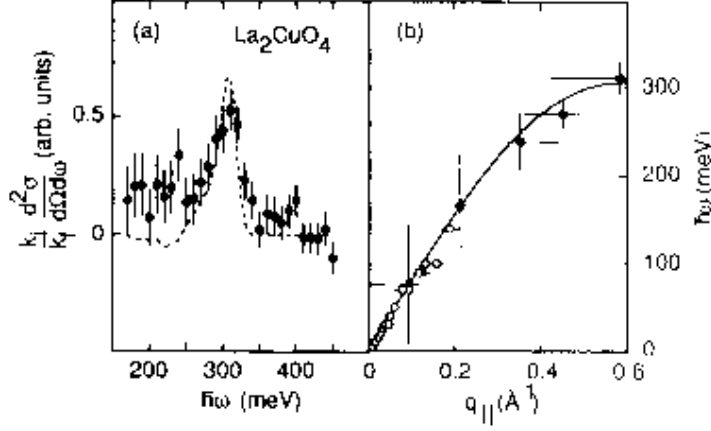


Figure 8: a) Inelastic neutron scattering intensity vs. energy transfer at 296K near zone boundary  $Q = (1, k, 0.5)$  for oriented  $\text{LaCuO}_4$  crystals with Neél temperature 260K; b) spin-wave dispersion  $\omega_{\mathbf{q}}$  vs.  $q_{||}$ , where  $q_{||}$  is in-plane wavevector. (after Hayden et al. 1991)

The result is usually expressed in terms of a constant  $\beta$  defined by

$$E_0 \equiv -NJzS \left( S + \frac{\beta}{z} \right), \quad (70)$$

and  $\beta = 0.58$  for 3D and xxx for 2D.

Quantum fluctuations have the further effect of preventing the staggered magnetization from achieving its full saturated value of  $S$ , as in the classical Neél state, as shown first by Anderson.<sup>23</sup> Let us consider the average  $z$ -component of spin in equilibrium at temperature  $T$ , averaging only over spins on sublattice  $A$  of a  $D$ -dimensional hypercubic lattice. From (60), we have  $\langle \hat{S}_z^A \rangle = S - N^{-1} \sum_{\mathbf{k}} \langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle$  within linear spin wave theory. Inverting the transformation (65), we can express the  $A$ 's in terms of the  $\alpha$ 's and  $\beta$ 's, whose averages we can easily calculate. Note the 0th order in  $1/S$  gives the classical result,  $\langle \hat{\mathbf{S}}_z^A \rangle$ , and the deviation is

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<sup>23</sup>P.W. Anderson, Phys. Rev. 86, 694 (1952).

the spin wave reduction of the sublattice moment

$$\begin{aligned}
\frac{\delta M_A}{N} &= \langle \hat{S}_z^A \rangle - S = -\frac{1}{N} \sum_{\mathbf{k}} \langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle \\
&= -\frac{1}{N} \sum_{\mathbf{k}} \langle (u_{\mathbf{k}} \alpha_{\mathbf{k}}^\dagger + v_{\mathbf{k}} \beta_{\mathbf{k}})(u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger) \rangle \\
&= -\frac{1}{N} \sum_{\mathbf{k}} u_{\mathbf{k}}^2 \langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} \rangle,
\end{aligned} \tag{71}$$

where  $N$  is the number of spins on sublattice  $B$ . We have neglected cross terms like  $\langle \alpha_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}^\dagger \rangle$  because the  $\alpha$  and  $\beta$  are independent quanta by construction. However the diagonal averages  $\langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} \rangle$  and  $\langle \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} \rangle$  are the expectation values for the number operators of independent bosons with dispersion  $\omega_{\mathbf{k}}$  in equilibrium, and so can be replaced (within linear spin wave theory) by

$$n_{\mathbf{k}} \equiv \langle \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} \rangle = \langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} \rangle = b(\omega_{\mathbf{k}}), \tag{72}$$

where  $b$  is the Bose distribution function. The tranformation coefficients  $u_{\mathbf{k}} = \cosh \theta_{\mathbf{k}}$  and  $v_{\mathbf{k}} = \sinh \theta_{\mathbf{k}}$  are determined by the condition (66) such that

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = \cosh 2\theta_{\mathbf{k}} = \frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}^2}} \tag{73}$$

$$v_{\mathbf{k}}^2 = \frac{1}{2} \left( \frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}^2}} - 1 \right), \tag{74}$$

such that the sublattice magnetization (71) becomes

$$\boxed{\frac{\delta M_A}{N} = \frac{1}{2} - \frac{1}{N} \sum_{\mathbf{k}} \left( n_{\mathbf{k}} + \frac{1}{2} \right) \frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}^2}}} \tag{75}$$

Remarks:

1. The correction  $\delta M_A$  is independent of  $S$ , and negative as it must be (see next point). However relative to the leading classical term  $S$  it becomes smaller and smaller as  $S$  increases, as expected.
2. The integral in (75) depends on the dimensionality of the system. It has a  $T$ -dependent part coming from  $n_{\mathbf{k}}$  and a  $T$ -independent part coming from the  $1/2$ . At  $T = 0$ , where there are no spin waves excited thermally,  $n_{\mathbf{k}} = 0$ , and we find

$$\frac{\delta M_A}{N} \simeq \begin{cases} -0.078 & D = 3 \\ -0.196 & D = 2 \\ \infty & D = 1 \end{cases} \quad (76)$$

The divergence in  $D = 1$  indicates the failure of spin-wave theory in one dimension, as discussed further in section xxx.

3. The low temperature behavior of  $\delta M(T)$  must be calculated carefully due to the singularities of the bose distribution function when  $\omega_k \rightarrow 0$ . If this divergence is cut off by introducing a scale  $k_0$  near  $\mathbf{k} = 0$  and  $\mathbf{k} = (\pi/a, \pi/a)$ , one finds that  $\delta M_A$  diverges as  $1/k_0$  in 1D, and as  $\log k_0$  in 2D, whereas it is finite as  $\mathbf{k}_0 \rightarrow 0$  in 3D. Thus on this basis one does not expect long range spin order at any nonzero temperature in two dimensions (see discussion of Mermin-Wagner theorem below), nor even at  $T = 0$  in one dimension.

### 3.4.3 Nonlinear spin wave theory

### 3.4.4 Frustrated models

## 3.5 1D & 2D Heisenberg magnets

### 3.5.1 Mermin-Wagner theorem

### 3.5.2 1D: Bethe solution

### 3.5.3 2D: Brief summary

## 3.6 Itinerant magnetism

“Itinerant magnetism” is a catch-all phrase which refers to magnetic effects in metallic systems (i.e., with conduction electrons). Most of the above discussion assumes that the spins which interact with each other are *localized*, and there are no mobile electrons. However we may study systems in which the electrons which magnetize, or nearly magnetize are mobile, and situations in which localized impurity spins interact with conduction electron spins in a host metal. The last problem turns out to be a very difficult many-body problem which stimulated Wilson to the develop of renormalization group ideas.

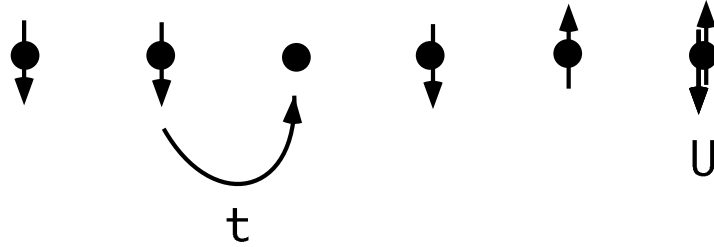
## 3.7 Stoner model for magnetism in metals

The first question is, can we have ferromagnetism in metallic systems with only one relevant band of electrons. The answer is yes, although the magnetization/electron in the ferromagnetic state is typically reduced drastically with respect to insulating ferromagnets. The simplest model which apparently describes this

kind of transition (there is no exact solution in  $D > 1$ ) is the Hubbard model we have already encountered. A great deal of attention has been focussed on the Hubbard model and its variants, particularly because it is the simplest model known to display a metal-insulator (Mott-Hubbard) transition qualitatively similar to what is observed in the high temperature superconductors. To review, the Hubbard model consists of a lattice of sites labelled by  $i$ , on which electrons of spin  $\uparrow$  or  $\downarrow$  may sit. The kinetic energy term in the Hamiltonian allows for electrons to hop between sites with matrix element  $t$ , and the potential energy simply requires an energy cost  $U$  every time two opposing spins occupy the same site.<sup>24</sup> Longer range interactions are neglected:

$$H = -t \sum_{\sigma} \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} U \sum_{\sigma} n_{i\sigma} n_{i-\sigma}, \quad (77)$$

where  $\langle ij \rangle$  means nearest neighbors only.



In its current form the kinetic energy, when Fourier transformed, corresponds, to a tight binding band in  $d$  dimensions of width  $4dt$ ,

$$\epsilon_k = -2t \sum_{\alpha=1}^d \cos k_{\alpha} a, \quad (78)$$

---

<sup>24</sup>What happened to the long-range part of the Coulomb interaction? Now that we know it is screened, we can hope to describe its effects by including only its matrix elements between electrons in wave functions localized on site  $i$  and site  $j$ , with  $|i - j|$  smaller than a screening length. The largest element is normally the  $i = j$  one, so it is frequently retained by itself. Note the Hamiltonian (77) includes only an on-site interaction for opposite spins. Of course like spins are forbidden to occupy the same site anyway by the Pauli principle.

where  $a$  is the lattice constant. The physics of the model is as follows. Imagine first that there is one electron per site, i.e. the band is half-filled. If  $U = 0$  the system is clearly metallic, but if  $U \rightarrow \infty$ , double occupation of sites will be “frozen out”. Since there are no holes, electrons cannot move, so the model must correspond to an insulating state; at some critical  $U$  a metal-insulator transition must take place. We are more interested in the case away from half-filling, where the Hubbard model is thought for large  $U$  and small doping (deviation of density from 1 particle/site) to have a ferromagnetic ground state.<sup>25</sup> In particular, we would like to investigate the transition from a *paramagnetic* to a *ferromagnetic* state as  $T$  is lowered.

This instability must show up in some quantity we can calculate. In a ferromagnet the susceptibility  $\chi$  diverges at the transition, i.e. the magnetization produced by the application of an infinitesimal external field is suddenly finite. In many-body language, the static, uniform spin susceptibility is the retarded spin density – spin density correlation function, (for the discussion below I take  $g\mu_B = 1$ )

$$\chi = \chi(q = 0, \omega = 0) = \lim_{h_z \rightarrow 0} \frac{\langle S_z \rangle}{h_z} = \int d^3r \int_0^\infty dt \langle [S_z(r, t), S_z(0, 0)] \rangle, \quad (79)$$

where in terms of electron number operators  $n_\sigma = \psi_\sigma^\dagger \psi_\sigma$ , the magnetization operators are  $S_z = (1/2)[n_\uparrow - n_\downarrow]$ , i.e. they just measure the surplus of up over down spins at some point in space.

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<sup>25</sup>At 1/2-filling, one electron per site, a great deal is known about the Hubbard model, in particular that the system is metallic for small  $U$  (at least for non-nested lattices, otherwise a narrow-gap spin density wave instability is present), but that as we increase  $U$  past a critical value  $U_c \sim D$  a transition to an antiferromagnetic insulating state occurs (Brinkman-Rice transition). With one single hole present, as  $U \rightarrow \infty$ , the system is however ferromagnetic (Nagaoka state).

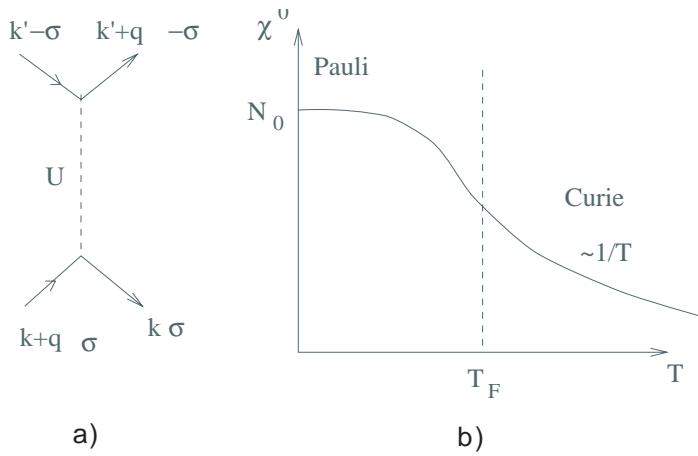


Figure 9: 1a) Hubbard interaction; 1b) Spin susceptibility vs.  $T$  for free fermions.

Diagrammatically, the Hubbard interaction  $H_{int} = U \sum_i n_{i\uparrow} n_{i\downarrow}$  looks like figure 9a); note only electrons of opposite spins interact. The magnetic susceptibility is a correlation function similar to the charge susceptibility we have already calculated. At time  $t=0$ , we measure the magnetization  $S_z$  of the system, allow the particle and hole thus created to propagate to a later time, scatter in all possible ways, and remeasure  $S_z$ . The so-called “Stoner model” of ferromagnetism approximates the perturbation series by the RPA form we have already encountered in our discussion of screening,<sup>26</sup> which gives  $\chi = \chi_0 / (1 - U\chi_0)$ . At sufficiently high  $T$  ( $\chi_0$  varies as  $1/T$  in the nondegenerate regime, Fig. 9c)) we will have  $U\chi_0(T) < 1$ , but as  $T$  is lowered,  $U\chi_0(T)$  increases. If  $U$  is large enough, such that  $UN_0 > 1$ , there will be a transition at  $U\chi_0(T_c) = 1$ , where  $\chi$  diverges. Note for  $U\chi_0(T) > 1$  ( $T < T_c$ ), the susceptibility is negative, so the model is unphysical in this region. This problem arises in part because the ferromagnetic state has a spontaneously broken symmetry,  $\langle S_z \rangle \neq 0$  even for

<sup>26</sup>In the static, homogeneous case it is equivalent to the self-consistent field (SCF) method of Weiss.

$h_z \rightarrow 0$ . Nevertheless the approach to the transition from above and the location of the transition appear qualitatively reasonable.

It is also interesting to note that for  $U\chi(0) = UN_0 < 1$ , there will be no transition, but the magnetic susceptibility will be enhanced at low temperatures. So-called “nearly ferromagnetic” metals like Pd are qualitatively described by this theory. Comparing the RPA form

$$\chi = \frac{\chi_0(T)}{1 - U\chi_0(T)} \quad (80)$$

to the free gas susceptibility in Figure 9b, we see that the system will look a bit like a free gas with enhanced density of states, and reduced degeneracy temperature  $T_F^*$ .<sup>27</sup> For Pd, the Fermi temperature calculated just by counting electrons works out to 1200K, but the susceptibility is found experimentally to be  $\sim 10\times$  larger than  $N_0$  calculated from band structure, and the susceptibility is already Curie-like around  $T \sim T_F^* \simeq 300\text{K}$ .

### 3.7.1 Moment formation in itinerant systems

We will be interested in asking what happens when we put a localized spin in a metal, but first we should ask how does that local moment form in the first place. If an arbitrary impurity is inserted into a metallic host, it is far from clear that any kind of localized moment will result: a donor electron could take its spin and wander off to join the conduction sea, for example. Fe impurities are known to give rise to a Curie term in the susceptibility when embedded in Cu, for example, but not in Al, suggesting

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<sup>27</sup>Compare to the Fermi liquid form

$$\chi = \frac{m^*}{m} \frac{\chi_0}{1 + F_0^a}. \quad (81)$$



that a moment simply does not form in the latter case. Anderson<sup>28</sup> showed under what circumstances an impurity level in an interacting host might give rise to a moment. He considered a model with a band of electrons<sup>29</sup> with energy  $\epsilon_{\mathbf{k}}$ , with an extra dispersionless impurity level  $E_0$ . Suppose there are strong local Coulomb interactions on the impurity site, so that we need to add a Hubbard-type repulsion. And finally suppose the conduction (d) electrons can hop on and off the impurity with some matrix element  $V$ . The model then looks like

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + E_0 \sum_{\sigma} n_{0\sigma} + V \sum_{\mathbf{k}\sigma} (c_{\mathbf{k}\sigma}^\dagger c_0 + c_0^\dagger c_{\mathbf{k}\sigma}) + \frac{1}{2} U \sum_{\sigma} n_{0\sigma} n_{0-\sigma}, \quad (82)$$

where  $n_{0\sigma} = c_{0\sigma}^\dagger c_{0\sigma}$  is the number of electrons of spin  $\sigma$  on the impurity site 0. By the Fermi Golden rule the decay rate due to scattering from the impurity of a band state  $\epsilon$  away from the Fermi level  $E_F$  *in the absence of the interaction*  $U$  is of order

$$\Delta(\epsilon) = \pi V^2 \sum_k \delta(\epsilon - \epsilon_{\mathbf{k}}) \simeq \pi V^2 N_0 \quad (83)$$

In the “Kondo” case shown in the figure, where  $E_0$  is well below the Fermi level, the scattering processes take place with electrons at the Fermi level  $\epsilon = 0$ , so the bare width of the impurity state is also  $\Delta \simeq \pi V^2 N_0$ . So far we still do not have a magnetic moment, since, in the absence of the interaction  $U$ , there would be an occupation of 2 antiparallel electrons. If one could effectively prohibit double occupancy, however, i.e. if  $U \gg \Delta$ , a single spin would remain in the localized with a net moment. Anderson

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<sup>28</sup>PW Anderson, Phys. Rev. 124, 41 (1961)

<sup>29</sup>The interesting situation for moment formation is when the bandwidth of the “primary” cond. electron band overlapping the Fermi level is much larger than the bare hybridization width of the impurity state. The two most commonly considered situations are a band of  $s$  electrons with  $d$ -level impurity (transition metal series) and  $d$ -electron band with localized  $f$ -level (rare earths/actinides-heavy fermions).

obtained the basic physics (supression of double occupancy) by doing a Hartree-Fock decoupling of the interaction  $U$  term. Schrieffer and Wolff in fact showed that in the limit  $U \rightarrow -\infty$ , the virtual charge fluctuations on the impurity site (occasional double occupation) are eliminated, and the only degree of freedom left (In the so-called Kondo regime corresponding to Fig. 10a) is a localized spin interacting with the conduction electrons via an effective Hamiltonian

$$\mathcal{H}_{Kondo} = J\mathbf{S} \cdot \boldsymbol{\sigma}, \quad (84)$$

where  $J$  is an antiferromagnetic exchange expressed in terms of the original Anderson model parameters as

$$J = 2\frac{V^2}{E_0}, \quad (85)$$

$S$  is the impurity spin-1/2, and

$$\sigma_i = \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\alpha\beta} c_{\mathbf{k}\alpha}^\dagger (\tau_i)_{\alpha\beta} c_{\mathbf{k}'\beta}, \quad (86)$$

with  $\tau_i$  the Pauli matrices, is just the conduction electron spin density at the impurity site.

### 3.7.2 RKKY Interaction

Kittel p. 360 et seq.

### 3.7.3 Kondo model

The Hartree-Fock approach to the moment formation problem was able to account for the existence of local moments at defects

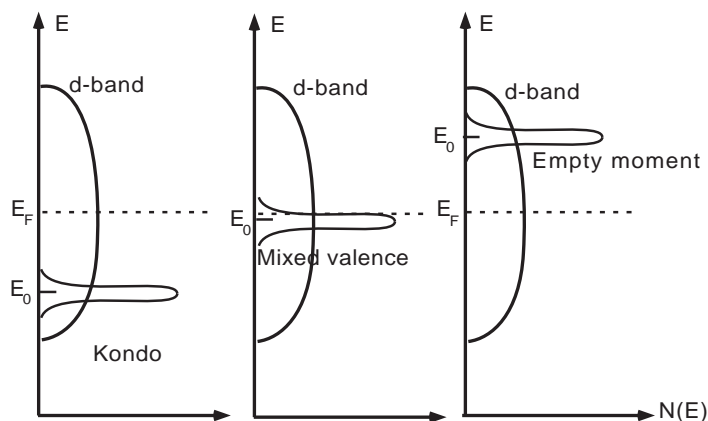


Figure 10: Three different regimes of large  $U$  Anderson model depending on position of bare level  $E_0$ . In Kondo regime ( $E_0 \ll E_F$ ), large moments form at high  $T$  but are screened at low  $T$ . In mixed valent regime, occupancy of impurity level is fractional and moment formation is marginal. For  $E_0 > E_F$ , level is empty and no moment forms.

in metallic hosts, in particular for large Curie terms in the susceptibility at high temperatures. What it did not predict, however, was that the low-temperature behavior of the model was very strange, and that in fact the moments present at high temperatures *disappear* at low temperatures, i.e. are screened completely by the conduction electrons, one of which effectively binds with the impurity moment to create a local singlet state which acts (at  $T = 0$ ) like a nonmagnetic scatterer. This basic physical picture had been guessed at earlier by J. Kondo,<sup>30</sup> who was trying to explain the existence of a resistance minimum in certain metallic alloys. Normally the resistance of metals is monotonically decreasing as the temperature is lowered, and adding impurities gives rise to a constant offset (Matthiesen's Rule) which does not change the monotonicity. For Fe in Cu, however, the impurity contribu-

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<sup>30</sup>J. Kondo, Prog. Theor. Phys. 32, 37 (64).

tion  $\delta\rho_{imp}$  *increased* as the temperature was lowered, and eventually saturated. Since Anderson had shown that Fe possessed a moment in this situation, Kondo analyzed the problem perturbatively in terms of a magnetic impurity coupling by exchange to a conduction band, i.e. adopted Eq. (84) as a model. Imagine that the system at  $t = -\infty$  consists of a Fermi sea  $|0\rangle$  and one additional electron in state  $|\mathbf{k}, \sigma\rangle$  at the Fermi level. The impurity spin has initial spin projection  $M$ , so we write the initial state as  $|i\rangle = c_{\mathbf{k}\sigma}^\dagger |0; M\rangle$ . Now turn on an interaction  $\mathcal{H}_1$  adiabatically and look at the scattering amplitude<sup>31</sup>

between  $|i\rangle$  and  $|f\rangle = c_{\mathbf{k}'\sigma'}^\dagger |0; M'\rangle$

$$\langle f|T|i\rangle = -2\pi i \langle f|\mathcal{H}_1 + \mathcal{H}_1 \frac{1}{\epsilon_{\mathbf{k}} - \mathcal{H}_0} \mathcal{H}_1 + \dots |i\rangle \quad (90)$$

If  $\mathcal{H}_1$  were just ordinary impurity (potential) scattering, we would have  $\mathcal{H}_1 = \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} c_{\mathbf{k}\sigma}^\dagger V_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}'\sigma'}$ , and there would be two distinct second-order processes  $\mathbf{k} \rightarrow \mathbf{k}'$  contributing to Eq. (90), as shown schematically at the top of Figure 11, of type a),

$$\langle 0|c_{\mathbf{k}'}c_{\mathbf{k}'}^\dagger V_{\mathbf{k}'\mathbf{p}}c_{\mathbf{p}} \frac{1}{\epsilon_{\mathbf{k}} - \mathcal{H}_0} c_{\mathbf{p}}^\dagger V_{\mathbf{p}\mathbf{k}} c_{\mathbf{k}} c_{\mathbf{k}}^\dagger |0\rangle = V_{\mathbf{k}'\mathbf{p}} \frac{1 - f(\epsilon_{\mathbf{p}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} V_{\mathbf{p}\mathbf{k}} \quad (91)$$

---

<sup>31</sup>Reminder: when using Fermi's Golden Rule (see e.g., Messiah, Quantum Mechanics p.807):

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar v} |T|^2 \rho(E) \quad (87)$$

we frequently are able to get away with replacing the full  $T$ -matrix by its perhaps more familiar 1st-order expansion

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar v} |\mathcal{H}_1|^2 \rho(E) \quad (88)$$

(Recall the  $T$  matrix is defined by  $\langle \phi_f|T|\phi_i\rangle = \langle \phi_f|T|\psi_i^+\rangle$ , where the  $\phi$ 's are plane waves and  $\psi^+$  is the scattering state with outgoing boundary condition.) In this case, however, we will not find the interesting  $\log T$  divergence until we go to 2nd order! So we take matrix elements of

$$T = \mathcal{H}_1 + \mathcal{H}_1 \frac{1}{\epsilon_{\mathbf{k}} - \mathcal{H}_0} \mathcal{H}_1 + \dots \quad (89)$$

This is equivalent and, I hope, clearer than the transition amplitude I calculated in class.

and type b),

$$\begin{aligned}
\langle 0 | c_{\mathbf{k}'} c_{\mathbf{p}}^\dagger V_{\mathbf{p}\mathbf{k}} c_{\mathbf{k}} & \frac{1}{\epsilon_{\mathbf{k}} - \mathcal{H}_0} c_{\mathbf{k}'}^\dagger V_{\mathbf{k}'\mathbf{p}} c_{\mathbf{p}} c_{\mathbf{k}}^\dagger | 0 \rangle \\
&= -V_{\mathbf{p}\mathbf{k}} \frac{f(\epsilon_{\mathbf{p}})}{\epsilon_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}} + \epsilon_{\mathbf{k}'})} V_{\mathbf{k}'\mathbf{p}} \\
&= V_{\mathbf{p}\mathbf{k}} \frac{f(\epsilon_{\mathbf{p}})}{\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{p}}} V_{\mathbf{k}'\mathbf{p}} \tag{92}
\end{aligned}$$

where I have assumed  $\mathbf{k}$  is initially occupied, and  $\mathbf{k}'$  empty, with  $\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}'}$ , whereas  $\mathbf{p}$  can be either; the equalities then follow from the usual application of  $c^\dagger c$  and  $cc^\dagger$  to  $|0\rangle$ . Careful checking of the order of the  $c$ 's in the two matrix elements will show you that the first process only takes place if the intermediate state  $\mathbf{p}$  is unoccupied, and the second only if it is unoccupied.

Now when one sums the two processes, the Fermi function cancels. This means there is no significant  $T$  dependence to this order ( $\rho_{imp}$  due to impurities is a constant at low  $T$ ), and thus the exclusion principle does not play an important role in ordinary potential scattering.

Now consider the analagous processes for spin-scattering. The perturbing Hamiltonian is Eq. 84. Let's examine the amplitude for *spin-flip* transitions caused by  $\mathcal{H}_1$ , first of type a),

$$\begin{aligned}
& \langle 0M_{s'} | \mathcal{H}_1 | 0M_s \rangle \tag{93} \\
&= \frac{J^2}{4} S_\mu S_\nu \langle 0M_{s'} | c_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}^\dagger \tau_{\sigma'\sigma''}^\nu c_{\mathbf{p}\sigma''} \frac{1}{\epsilon_{\mathbf{k}} - \mathcal{H}_0} c_{\mathbf{p}\sigma''}^\dagger \tau_{\sigma''\sigma}^\mu c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger | 0M_s \rangle \\
&= \frac{J^2}{4} \frac{1 - f(\epsilon_{\mathbf{p}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} \langle M'_S | S_\nu S_\mu \tau_{\sigma'\sigma''}^\nu \tau_{\sigma''\sigma}^\mu | M_S \rangle
\end{aligned}$$

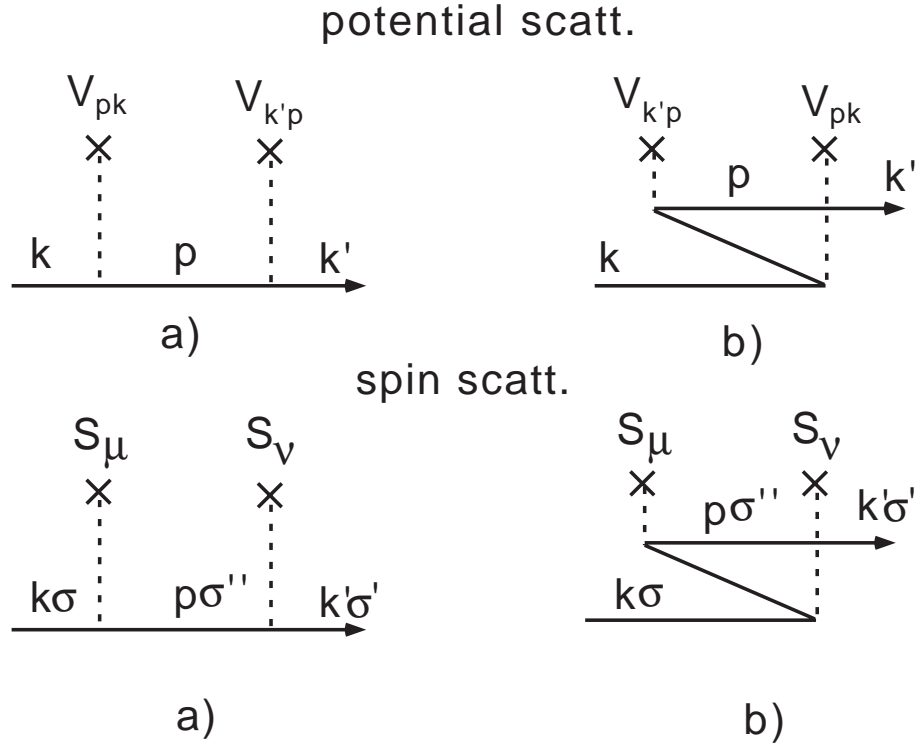


Figure 11: 2nd-order scattering processes: a) direct and b) exchange scattering. Top: potential scattering; bottom: spin scattering. Two terms corresponding to Eq. 90

and then of type b),

$$\frac{J^2}{4} \frac{f(\epsilon_{\mathbf{p}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} \langle M'_S | S_\nu S_\mu \tau_{\sigma'\sigma''}^\nu \tau_{\sigma'\sigma''}^\mu | M_S \rangle. \quad (94)$$

Now note that  $\tau_{\sigma'\sigma''}^\mu \tau_{\sigma'\sigma''}^\nu = (\tau^\mu \tau^\nu)_{\sigma'\sigma}$ , and use the identity  $\tau_\mu \tau_\nu = \delta_{\mu\nu} + i\tau_\alpha \epsilon_{\alpha\mu\nu}$ . The  $\delta_{\mu\nu}$  pieces clearly will only give contributions proportional to  $\mathbf{S}^2$ , so they aren't the important ones which will distinguish between a) and b) processes compared to the potential scattering case. The  $\epsilon_{\alpha\nu\mu}$  terms give results of differing sign, since a) gives  $\epsilon_{\alpha\nu\mu}$  and b) gives  $\epsilon_{\alpha\mu\nu}$ . Note the basic difference between the 2nd-order potential scattering and spin scattering is that the matrix elements in the spin scattering case, i.e. the  $S_\mu$ , didn't commute! When we add a) and b) again the result is

$$\begin{aligned} \frac{J^2}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} \left\{ \left[ \frac{1}{4} S(S+1) - \langle M'_S \sigma' | \mathbf{S} \cdot \sigma | M_S, \sigma \rangle \right] \right. \\ \left. + f(\epsilon_{\mathbf{p}}) \langle M'_S \sigma' | \mathbf{S} \cdot \sigma | M_S, \sigma \rangle \right\} \quad (95) \end{aligned}$$

so the spin-scattering amplitude does depend on  $T$  through  $f(\epsilon_{\mathbf{p}})$ . Summing over the intermediate states  $\mathbf{p}\sigma''$  gives a factor

$$\begin{aligned} \sum_{\mathbf{p}} \frac{f(\epsilon_{\mathbf{p}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} &\simeq N_0 \int d\xi_{\mathbf{p}} \frac{f(\xi_{\mathbf{p}})}{\xi_{\mathbf{k}} - \xi_{\mathbf{p}}} \\ &= N_0 \int d\xi_{\mathbf{p}} \left( -\frac{\partial f}{\partial \xi_{\mathbf{p}}} \right) \log |\xi_{\mathbf{k}} - \xi_{\mathbf{p}}|, \end{aligned} \quad (96)$$

which is of order  $\log T$  for states  $\xi_{\mathbf{k}}$  at the Fermi surface! Thus the spin part of the interaction, to a first approximation, makes a contribution to the resistance of order  $J^3 \log T$  ( $\rho$  involves the square of the scattering amplitude, and the cross terms between the 1st and 2nd-order terms in perturbation theory give this result). Kondo pointed to this result and said, “Aha!”, here is a contribution which gets big as  $T$  gets small. However this can’t be the final answer. The divergence signals that perturbation theory is breaking down, so this is one of those very singular problems where we have to find a way to sum all the processes. We have discovered that the Kondo problem, despite the fact that only a single impurity is involved, is a complicated many-body problem. Why? Because the spin induces correlations between the electrons in the Fermi sea. Example: suppose two electrons, both with spin up, try to spin flip scatter from a spin-down impurity. The first electron can exchange its spin with the impurity and leave it spin up. The second electron therefore cannot spin-flip scatter by spin conservation. Thus the electrons of the conduction band can’t be treated as independent objects.

Summing an infinite subset of the processes depicted in Figure 11 or a variety of other techniques give a picture of a singlet bound state where the impurity spin binds one electron from the

conduction electron sea with binding energy

$$T_K = D e^{-1/(JN_0)}, \quad (97)$$

where  $D$  is the conduction electron bandwidth. The renormalization group picture developed by Wilson in the 70s and the exact Bethe ansatz solution of Wiegman/Tsvelick and Andrei/Lowenstein in 198? give a picture of a free spin at high temperatures, which hybridizes more and more strongly with the conduction electron sea as the temperature is lowered. Below the singlet formation temperature of  $T_K$ , the moment is screened and the impurity acts like a potential scatterer with large phase shift, which approaches  $\pi/2$  at  $T = 0$ .



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## Reading:

1. Ch. 26, Ashcroft & Mermin
2. Ch. 7, Kittel

# 4 Electron-phonon interaction

## 4.1 Hamiltonian

The subtle interplay of electrons and phonons was explained in the 50's by some of the earliest practitioners of quantum many-body theory, leading eventually to an understanding of the mechanism underlying superconductivity. Recall that the ions in a metal have two basic effects on the electronic states: 1) the *static* ionic lattice provides a periodic potential in which conduction electrons must move, leading to the evolution of plane wave states in the Fermi gas into Bloch waves in the crystal, and 2) the scattering of electrons by lattice *vibrations*, and vice versa. The first effect will be ignored here, as we are essentially interested in long-wavelength phenomena, where the differences between proper calculations using Bloch waves and simpler ones using plane waves are negligible. It suffices then to consider the phonons in a lattice interacting with a Fermi gas in which the most important effects of the long-range Coulomb interaction have been accounted for. *Without* the Coulomb interaction, the phonon frequencies are just those we would get from a classical model of balls of mass  $M$  (ionic mass) connected by springs. For a 3D solid with 1 atom per unit cell, there are  $3N$  normal modes comprising 3 *acoustic* phonon branches  $\omega_k^\lambda$ . When one includes the long-range Coulomb interaction but neglects the electron-phonon coupling, one finds

that the longitudinal acoustic mode has been lifted to the ionic plasma frequency,  $\omega_{pl}^{ion} \simeq (4\pi Z^2 e^2 n / M)^{1/2}$ . The terms of the Goldstone theorem which insists on the existence of an acoustic mode for each spontaneously broken continuous symmetry are violated by the long-range nature of the Coulomb force, and the sloshing back and forth of the ion “fluid” at  $\omega_{pl}^{ion}$  occurs for the same reason and at the same frequency (up to the mass difference) that it does in the electron case. At this point we are seriously worried that we don’t understand how acoustic phonons ever exist in charged systems. If one now includes the electron-phonon coupling, however, the electronic medium screens the long-range Coulomb interaction, leading to a finite interaction length and the recovery of the Goldstone (acoustic) mode.

Let’s give a brief overview of where we’re going. I first want to get to the point where we can write down the full Hamiltonian for the problem. We want to show that it makes sense to write the Hamiltonian describing the electron-phonon system as

$$H = H_{el}^0 + H_{ph}^0 + H_{coul} + H_{int}, \quad (1)$$

where

$$H_{el}^0 = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} \quad (2)$$

$$H_{ph}^0 = \sum_{k\lambda} \omega_{k\lambda} (a_{k\lambda}^\dagger a_{k\lambda} + \frac{1}{2}) \quad (3)$$

$$H_{Coul} = \frac{1}{2} \sum_{\substack{k k' q \\ \sigma \sigma'}} V(q) c_{k'+q\sigma'}^\dagger c_{k\sigma}^\dagger c_{k+q\sigma} c_{k'\sigma'} \quad (4)$$

$$H_{int} = \sum_{k k' \sigma \lambda} g_{k k'} c_{k\sigma}^\dagger c_{k'\sigma} (a_{-q\lambda}^\dagger + a_{q\lambda}) \quad (5)$$

where  $a_{k\lambda}^\dagger$  creates a phonon with wave vector  $q \equiv k' - k$  and polarization  $\lambda$ , and  $g_{k k'} \propto M^{-1/2}$  is the bare electron-phonon

coupling. The unperturbed phonon Hamiltonian  $H_{ph}$  is of course just the sum of  $3N$  independent harmonic oscillators in 2nd quantized form, and the bare Coulomb matrix element in  $H_{Coul}$  is  $V(q) = 4\pi e^2/q^2$ . The derivation of the electron-phonon Hamiltonian  $H_{int}$  and its quantization is relatively straightforward, and I will sketch it here.

#### 4.1.1 Derivation of $e^-$ -ph coupling

Assume the ion is located at position  $\mathbf{R}_i$ , at a displacement  $\mathbf{u}_i$  from its equilibrium position  $\mathbf{R}_i^0$ . If the potential of the ion is assumed to be rigid, the interaction energy of the electronic charge density with the ions is simply<sup>1</sup>

$$H_{int} = \sum_{i\sigma} \int d^3r \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r}) V(\mathbf{r} - \mathbf{R}_i). \quad (6)$$

For small amplitude vibrations, we can expand in powers of  $\mathbf{u}_i$ :

$$\begin{aligned} H_{int} = & \sum_{i\sigma} \int d^3r \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r}) V(\mathbf{r} - \mathbf{R}_i^0) \\ & + \sum_{i\sigma} \int d^3r \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r}) \mathbf{u}_i \cdot \nabla_{\mathbf{R}_i} V(\mathbf{r} - \mathbf{R}_i) |_{\mathbf{R}_i^0} + \dots \end{aligned} \quad (7)$$

Now expand the field operators  $\psi_\sigma$  in terms of Bloch waves:

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma} \phi_{\mathbf{k}}(\mathbf{r}), \quad (8)$$

where

$$\phi_{\mathbf{k}\sigma}(\mathbf{r} + \mathbf{R}_i^0) = e^{i\mathbf{k} \cdot \mathbf{R}_i^0} \phi_{\mathbf{k}}(\mathbf{r}) \quad (9)$$

so the quantity which appears in Eq. (7) may be recast by performing a shift by a Bravais lattice vector and using the periodicity

---

<sup>1</sup>This is for a Bravais lattice. If there is a basis one has to be a bit careful about labelling the lattice sites with additional intracell indices, i.e.  $\mathbf{R}_{i\alpha}$ ,  $\alpha = 1 \dots m$ , where  $m$  is number of atoms/cell.

of  $\nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0)$ ,

$$\begin{aligned} & \int d^3r \phi_{\mathbf{k}'\sigma}^*(\mathbf{r}) \phi_{\mathbf{k}\sigma}(\mathbf{r}) \nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0) \\ &= \int d^3r \phi_{\mathbf{k}'\sigma}^*(\mathbf{r} + \mathbf{R}_j^0) \phi_{\mathbf{k}\sigma}(\mathbf{r} + \mathbf{R}_j^0) \nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0) \\ &= e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_j^0} \underbrace{\int d^3r \phi_{\mathbf{k}'\sigma}^*(\mathbf{r}) \phi_{\mathbf{k}\sigma}(\mathbf{r}) \nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0)}_{\mathbf{W}_{\mathbf{k}\mathbf{k}'}} \end{aligned} \quad (10)$$

$$\mathbf{W}_{\mathbf{k}\mathbf{k}'} \quad (11)$$

Now let us 2nd-quantize the displacement  $\mathbf{u}$  as we did when we were discussing the isolated phonon system,<sup>2</sup>

$$\mathbf{u}_i(t) = \frac{1}{\sqrt{NM}} \sum_{\mathbf{k}\lambda} Q(\mathbf{k}, t) \mathbf{e}^\lambda(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}_i^0} \quad (13)$$

with

$$Q_\lambda(\mathbf{q}) = \frac{1}{\sqrt{2\omega_\lambda(\mathbf{q})}} \left( a_\lambda(\mathbf{q}) + a_\lambda^\dagger(-\mathbf{q}) \right) \quad (14)$$

so interaction Hamiltonian can be rewritten

$$\begin{aligned} H_{int} &= \sum_{\mathbf{k}\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}\sigma} \sum_j \mathbf{W}_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_j^0} \frac{1}{\sqrt{NM}} \times \\ &\quad \times \sum_{\mathbf{q}\lambda} Q_\lambda(\mathbf{q}) \mathbf{e}^\lambda(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{R}_j^0} \\ &= \sum_{\mathbf{k}\mathbf{k}'\sigma} \sum_{\lambda} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}\sigma} \left( \mathbf{W}_{\mathbf{k}\mathbf{k}'} \cdot \mathbf{e}^\lambda(\mathbf{q}) \right) Q_\lambda(\mathbf{q}) \sqrt{\frac{N}{M}} \\ &\equiv \sum_{\mathbf{k}\mathbf{k}'\sigma\lambda} g_{\mathbf{k}\mathbf{k}'\lambda} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}\sigma} \left( a_\lambda(\mathbf{q}) + a_\lambda^\dagger(-\mathbf{q}) \right) \end{aligned} \quad (15)$$

---

<sup>2</sup>Before we dealt primarily with the 1D chain, so I suppressed the polarization indices. It is important to recall that in a 3 dimensional system there are  $3N$  normal modes ( $3mN$  if there are  $m$  atoms per unit cell). For each value of  $\mathbf{k}$  there are 3 acoustic (optical only if there are add'l atoms per unit cell requiring index  $\alpha$ ) modes denoted by different values of the branch index  $\lambda$ . The vectors  $\mathbf{e}^\lambda(\mathbf{k})$  are the polarization vectors of the modes and satisfy the orthogonality condition

$$\sum_{\alpha} \mathbf{e}_{\alpha}^{\lambda}(\mathbf{k}) \cdot \mathbf{e}_{\alpha}^{\lambda'}(\mathbf{k}) = \delta_{\lambda\lambda'} \quad (12)$$

where now  $\mathbf{q}$  due to momentum conservation ( $\delta$ -function from summing over  $j$ ) is to be interpreted as

$$\mathbf{q} = \mathbf{k} - \mathbf{k}' + \mathbf{G} \quad (16)$$

with  $\mathbf{G}$  is a vector of reciprocal lattice (arose because  $\mathbf{q}$  was defined to lie in 1st B-zone). The electron-phonon coupling constant is

$$g_{\mathbf{k}\mathbf{k}'\lambda} = (\mathbf{W}_{\mathbf{k}\mathbf{k}'} \cdot \mathbf{e}^\lambda(\mathbf{q})) \sqrt{\frac{N}{2M\omega_{pl}^{ion}(\mathbf{q})}} \quad (17)$$

The final result, then, is that an electron in state  $\mathbf{k}, \sigma$  can undergo a scattering process with amplitude  $g_{\mathbf{k}\mathbf{k}'}$ , ending up in final state  $\mathbf{k}', \sigma$  by absorption (emission) of a phonon of momentum  $\mathbf{q}$ . This form is useful, but calculating  $g_{\mathbf{k}\mathbf{k}'}$  from first principles is difficult because  $V$  is poorly known.

#### 4.1.2 Jellium model

We can get some dimensionally reasonable results in the so-called "jellium" model, where the ions are represented as a featureless, positively charged elastic continuum,<sup>3</sup> we will simply replace the eigenfrequencies  $\omega_{k\lambda}$  of the neutral system by the constant  $\omega_{pl}^{ion}$  according to the arguments given above. Again we expand the crystal potential  $V(r - R_j)$  around the equilibrium sites  $R_i^0$ . The displacements  $\mathbf{u}(\mathbf{R})$  in the jellium gives a charge density fluctuation<sup>4</sup>  $-nZe\nabla \cdot \mathbf{u}$ . This interacts with the electron gas through the Coulomb interaction, leading to the interaction

$$H_{int}^{jellium} = Ze^2 \sum_{\sigma} \int d^3r d^3r' \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \frac{1}{|\mathbf{r} - \mathbf{r}'|} \nabla \cdot \mathbf{u}(\mathbf{r}'), \quad (18)$$

---

<sup>3</sup>... justified by the large masses and correspondingly long timescales for ionic motion (Born-Oppenheimer)

<sup>4</sup>Recall from E& M the polarization charge density is  $\rho_P = -\nabla \cdot \mathbf{P}$ , where  $\mathbf{P}$  is the polarization, and the polarization due to a density  $n$  of dipole moments  $\mathbf{p} = Ze\mathbf{u}$  is therefore  $nZe\mathbf{u}$ .

and then quantizing the ionic displacements  $u_i = R_i - R_i^0$  as in Eq.(13), one finds

$$H_{int}^{jellium} = \sum_{\mathbf{k}\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}\sigma} \left( a_\lambda(\mathbf{q}) + a_\lambda^\dagger(\mathbf{q}) \right) \frac{4\pi i \mathbf{q} \cdot \mathbf{e}_\lambda(\mathbf{q})}{M^{1/2}} \frac{Ze^2 n}{q^2} \quad (19)$$

Comparing with Eq. (15), we see that the effective e-ph coupling constant in an isotropic system is

$$\boxed{g(q) = \frac{4\pi i Z e^2 n^{1/2}}{q M^{1/2}}}. \quad (20)$$

#### 4.1.3 Screening.

The first point I would like to review is the renormalization of the electron-phonon coupling which leads to screening and the recovery of the acoustic spectrum. The main point is to realize that the singular behavior is due to the long-range Coulomb interaction, which will be screened. Any time a phonon of momentum  $q$  is excited, it creates charge density fluctuations because the ions are positively charged. These then interact with the electron gas. The bare potential created by the charge fluctuation is proportional to the electron-phonon coupling constant, so screening the ionic charge amounts to replacing the bare coupling  $g$  with a screened coupling

$$\bar{g}(q, \omega_n) = g(q)/\epsilon(q, \omega_n), \quad (21)$$

where  $q = k' - k$  and  $\epsilon(q, \omega_n) = 1 - V(q)\chi(q, \omega_n)$  is the RPA dielectric constant. The frequency dependence of the dielectric constant will become important for us on scales of the Debye frequency  $\omega_D$  or smaller, and this is normally a very small scale by

electronic standards! So for most purposes we keep a frequency-independent screened coupling  $\bar{g}(q) \simeq g(q)/\epsilon(q, 0)$ .

We would like to see that this screening recovers acoustic modes as observed and expected. The *bare* interaction Hamiltonian may be written in the Jellium model as (see Eq. (15))

$$H_{int} = \sum_q g(q) n_{-q} Q_q \quad (22)$$

with  $n_q = \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}}$ . Consider now the entire Hamiltonian for the phonon coordinates, including the coupling to the electron gas (recall derivation of normal modes for linear chain in Section 1):

$$H_{ph} + H_{int} = \frac{1}{2} \sum_{\mathbf{q}} \left( \frac{1}{M} P_{\mathbf{q}} P_{-\mathbf{q}} + M \omega_{pl}^{ion2} Q_{\mathbf{q}} Q_{-\mathbf{q}} + 2g_{\mathbf{q}} Q_{\mathbf{q}} n_{-\mathbf{q}} \right) \quad (23)$$

The Heisenberg equation of motion for the operator  $Q_{\mathbf{q}}$  becomes (check!)

$$\ddot{Q}_{\mathbf{q}} + \omega_{pl}^{ion2} Q_{\mathbf{q}} + g_{-\mathbf{q}} n_{\mathbf{q}} = 0 \quad (24)$$

We noted above that the ionic charge density fluctuation *induced* by an ionic displacement  $\mathbf{u}$  was  $en^{ion} = -nZe\nabla \cdot \mathbf{u}$ ; in Fourier space with Eq. (13) this reads

$$n_{\mathbf{q}}^{ion} = -iZ \sqrt{\frac{n}{M}} q Q_{\mathbf{q}} \quad (25)$$

Also recall the definition of the dielectric constant

$$\epsilon = \frac{\text{“external charge”}}{\text{total charge}}. \quad (26)$$

Now the total charge fluctuation is just electronic + ionic  $n_{\mathbf{q}} + n_{\mathbf{q}}^{ion}$ , so

$$n_{\mathbf{q}} = n_{\mathbf{q}}^{ion} (1 - 1/\epsilon) = -iZ \sqrt{\frac{n}{M}} q Q_{\mathbf{q}} (1 - 1/\epsilon) \quad (27)$$



$$= iZ\sqrt{\frac{n}{M}}qQ_{\mathbf{q}}\left(\frac{k_{TF}^2}{q^2 + k_{TF}^2}\right), \quad (28)$$

where in the last step we have used the Thomas-Fermi approximation for the dielectric function,  $\epsilon = 1 + k_{TF}^2/q^2$ .

$$\omega_{phonon}^2 = \omega_{pl}^{ion2} \left[ 1 - \frac{k_{TF}^2}{q^2 + k_{TF}^2} \right]. \quad (29)$$

Equation of motion becomes

$$\begin{aligned} 0 &= \ddot{Q}_{\mathbf{q}} + \omega_{pl}^{ion2} Q_{\mathbf{q}} + \underbrace{\left( \frac{4\pi i Z e^2 n^{1/2}}{q M^{\frac{1}{2}}} \right)}_{\text{Thomas-Fermi screening}} iZ\sqrt{\frac{n}{M}}qQ_{\mathbf{q}}\left(\frac{k_{TF}^2}{q^2 + k_{TF}^2}\right) \\ &= \ddot{Q}_{\mathbf{q}} + \omega_{pl}^{ion2} \left[ 1 - \left( \frac{k_{TF}^2}{q^2 + k_{TF}^2} \right) \right] Q_{\mathbf{q}}. \end{aligned} \quad (30)$$

So the phonon oscillation frequencies are

$$\omega_{phonon}^2 = \omega_{pl}^{ion2} \left( \frac{q^2}{q^2 + k_{TF}^2} \right) \quad (31)$$

Since  $k_{TF}^2 = 6\pi n e^2 / E_F$ , we do in fact recover *acoustic* phonons  $i\omega_n = cq$  as  $q \rightarrow 0$ , with speed

$$c = (m/3M)^{1/2} v_F. \quad (32)$$

So we have proven that sound propagates in a metal, which you already knew, but it is important to remember that screening makes it happen!

## 4.2 Polarons

## 4.3 Bloch resistivity

## 4.4 Effective $e^- - e^-$ interaction

For superconductivity it will be important to understand why one electron attracts each other effectively by polarizing the lattice. We now have at our disposal the effective screened electron-phonon interaction with coupling constant  $g_{\mathbf{k}\mathbf{k}'}$  and renormalized phonon frequencies  $\omega_\lambda(\mathbf{q})$ . An interaction between electrons must involve the 1st electron polarizing the lattice, and the second interacting with this polarization, i.e. it must be a 2nd-order process in the coupling constant  $g$ . We can represent these processes in terms of Feynman-type pictures: The amplitude of the first pro-

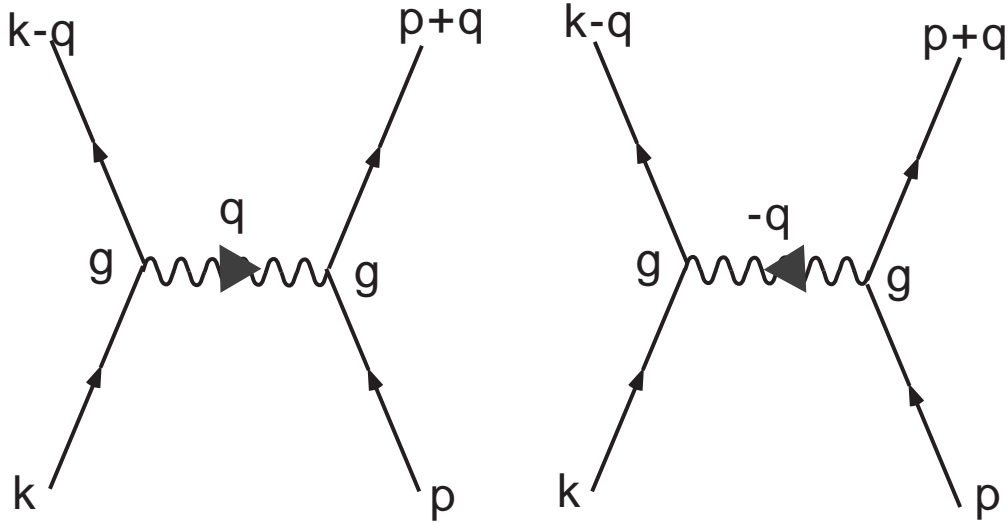


Figure 1: Electron-electron interaction due to phonon exchange. Straight lines are electrons, wiggly are phonons, vertices are e-ph coupling constants  $g$ .

cess, according to 2nd-order perturbation theory, where the 1st

electron emits a phonon, is

$$V_q^1 = \frac{|g_q|^2}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}}} \quad (33)$$

whereas for the process where it absorbs a phonon we get

$$V_q^2 = \frac{|g_q|^2}{\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}+\mathbf{q}} - \omega_{\mathbf{q}}}. \quad (34)$$

Note as usual we have energy conservation at every scattering event depicted in these processes, i.e.

$$\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{p}} = \epsilon_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{p}+\mathbf{q}} \quad (35)$$

and I've assumed  $\omega_{\mathbf{q}} = \omega_{-\mathbf{q}}$ . According to quantum mechanics the two amplitudes contribute additively:

$$V_q = V_q^1 + V_q^2 == \frac{|g_q|^2 \omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2 - \omega_{\mathbf{q}}^2}. \quad (36)$$

Let's analyze this expression for the “effective electron-electron interaction” qualitatively. We will primarily be interested in  $\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} \ll \omega_{\mathbf{q}}$ , since this situation corresponds to electrons with their momenta both quite close to the Fermi surface, well within a shell of width  $\omega_D$ , a typical phonon energy.

- attractive
- ind. of  $\mathbf{k} \Rightarrow$  isotropic
- rapidly decreases when  $\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} \sim \omega_D$ .
- energy space: interaction spread over  $\omega_D \Rightarrow$  in time space it's *retarded*
- comparable when spread over time to Coulomb interactions: some metals superconducting, some not.

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# 5 Superconductivity

## 5.1 Phenomenology

Superconductivity was discovered in 1911 in the Leiden laboratory of Kamerlingh Onnes when a so-called “blue boy” (local high school student recruited for the tedious job of monitoring experiments) noticed that the resistivity of *Hg* metal vanished abruptly at about 4K. Although phenomenological models with predictive power were developed in the 30’s and 40’s, the microscopic mechanism underlying superconductivity was not discovered until 1957 by Bardeen Cooper and Schrieffer. Superconductors have been studied intensively for their fundamental interest and for the promise of technological applications which would be possible if a material which superconducts at room temperature were discovered. Until 1986, critical temperatures ( $T_c$ ’s) at which resistance disappears were always less than about 23K. In 1986, Bednorz and Mueller published a paper, subsequently recognized with the 1987 Nobel prize, for the discovery of a new class of materials which currently include members with  $T_c$ ’s of about 135K.

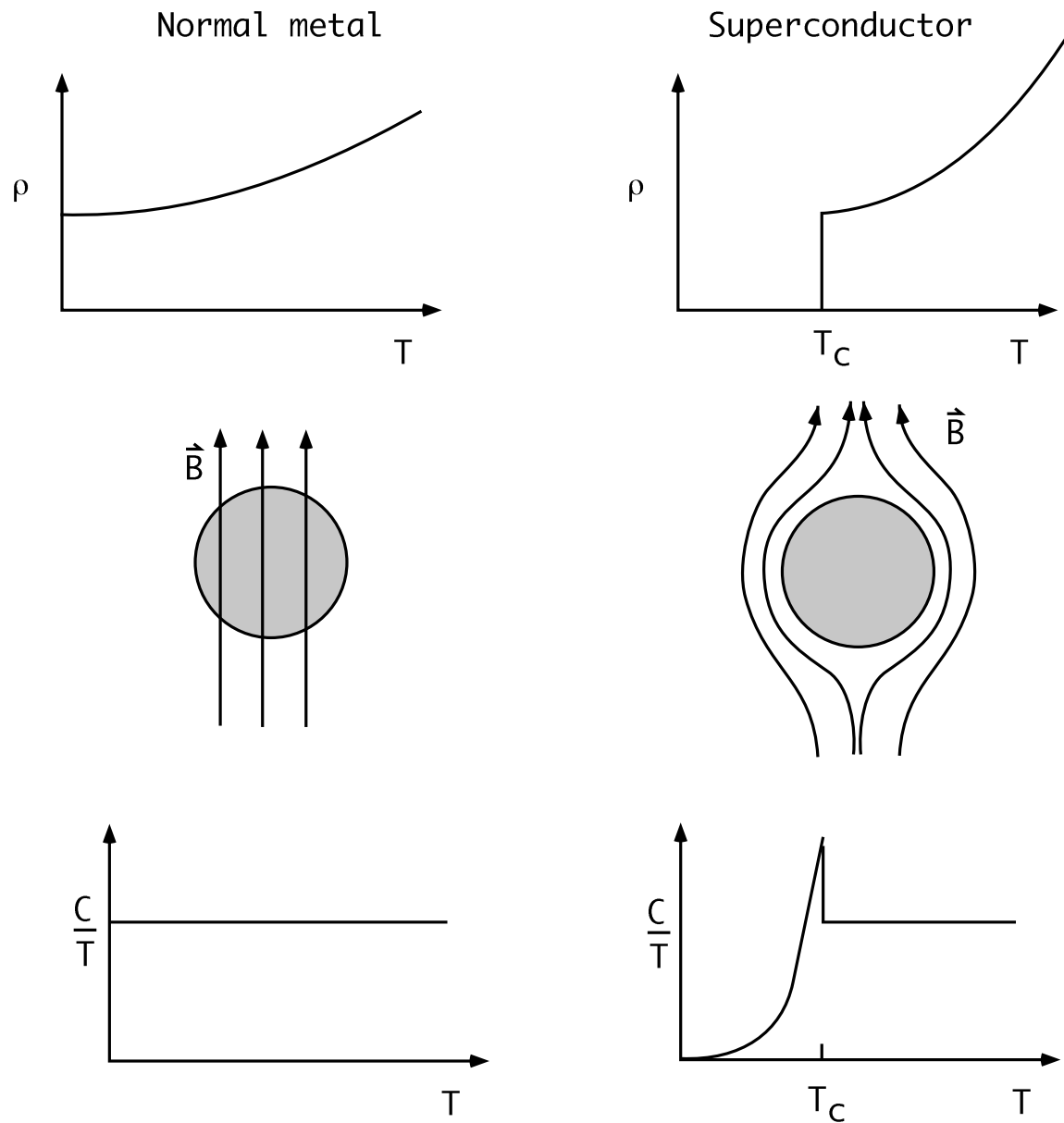


Figure 1: Properties of superconductors.

Superconducting materials exhibit the following unusual behaviors:

1. **Zero resistance.** Below a material's  $T_c$ , the DC electrical resistivity  $\rho$  is really zero, not just very small. This leads to the possibility of a related effect,
2. **Persistent currents.** If a current is set up in a superconductor with multiply connected topology, e.g. a torus,

it will flow forever without any driving voltage. (In practice experiments have been performed in which persistent currents flow for several years without signs of degrading).

3. **Perfect diamagnetism.** A superconductor expels a weak magnetic field nearly completely from its interior (screening currents flow to compensate the field within a surface layer of a few 100 or 1000 Å, and the field at the sample surface drops to zero over this layer).
4. **Energy gap.** Most thermodynamic properties of a superconductor are found to vary as  $e^{-\Delta/(k_B T)}$ , indicating the existence of a gap, or energy interval with no allowed eigenenergies, in the energy spectrum. Idea: when there is a gap, only an exponentially small number of particles have enough thermal energy to be promoted to the available unoccupied states above the gap. In addition, this gap is visible in electromagnetic absorption: send in a photon at low temperatures (strictly speaking,  $T = 0$ ), and no absorption is possible until the photon energy reaches  $2\Delta$ , i.e. until the energy required to break a pair is available.

## 5.2 Electron-phonon interaction

Superconductivity is due to an effective attraction between conduction electrons. Since two electrons experience a repulsive Coulomb force, there must be an additional attractive force between two electrons when they are placed in a metallic environment. In classic superconductors, this force

is known to arise from the interaction with the ionic system. In previous discussion of a normal metal, the ions were replaced by a homogeneous positive background which enforces charge neutrality in the system. In reality, this medium is polarizable—the number of ions per unit volume can fluctuate in time. In particular, if we imagine a snapshot of a single electron entering a region of the metal, it will create a net positive charge density near itself by attracting the oppositely charged ions. Crucial here is that a typical electron close to the Fermi surface moves with velocity  $v_F = \hbar k_F / m$  which is much larger than the velocity of the ions,  $v_I = V_F m / M$ . So by the time ( $\tau \sim 2\pi / \omega_D \sim 10^{-13}$  sec) the ions have polarized themselves, 1st electron is long gone (it's moved a distance  $v_F \tau \sim 10^8 \text{ cm/s} \sim 1000 \text{ \AA}$ ), and 2nd electron can happen by to lower its energy with the concentration of positive charge before the ionic fluctuation relaxes away. This gives rise to an effective attraction between the two electrons as shown, which may be large enough to overcome the repulsive Coulomb interaction. Historically, this electron-phonon “pairing” mechanism was suggested by Frölich in 1950, and confirmed by the discovery of the “isotope effect”, wherein  $T_c$  was found to vary as  $M^{-1/2}$  for materials which were identical chemically but which were made with different isotopes.

The simplest model for the total interaction between two electrons in momentum states  $\mathbf{k}$  and  $\mathbf{k}'$ , with  $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}'$ , interacting both by direct Coulomb and electron-phonon forces, is given by



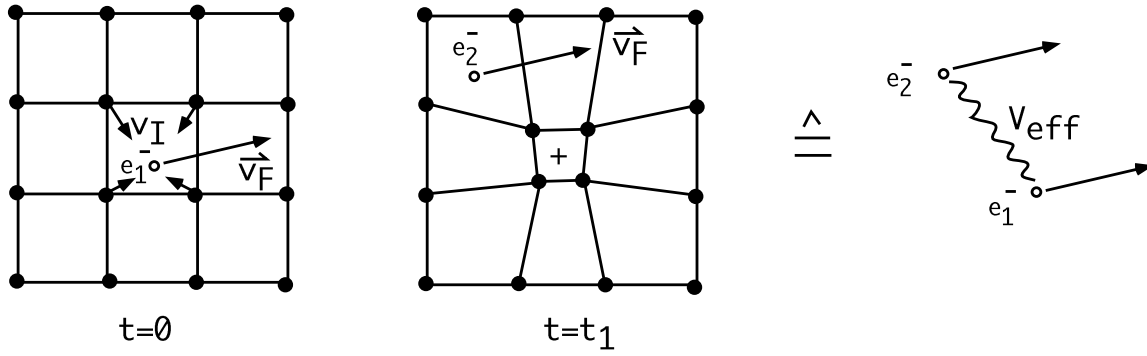


Figure 2: Effective attraction of two electrons due to “phonon exchange”

$$V(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2 + k_s^2} + \frac{4\pi e^2}{q^2 + k_s^2} \frac{\omega_q^2}{\omega^2 - \omega_q^2}, \quad (1)$$

in the jellium model. Here first term is Coulomb interaction in the presence of a medium with dielectric constant  $\epsilon = 1 + k_s^2/q^2$ , and  $\omega_q$  are the phonon frequencies. The screening length  $k_s^{-1}$  is  $1\text{\AA}$  or so in a good metal. Second term is interaction due to exchange of phonons, i.e. the mechanism pictured in the figure. Note it is frequency-dependent, reflecting the *retarded* nature of interaction (see figure), and in particular that the 2nd term is attractive for  $\omega < \omega_q \sim \omega_D$ . Something is not quite right here, however; it looks indeed as though the two terms are of the same order as  $\omega \rightarrow 0$ ; indeed they cancel each other there, giving  $V(\omega \rightarrow 0) = 0$ . Furthermore,  $V$  is always attractive at low frequencies, suggesting that all metals should be superconductors, which is not the case. These points indicate that the jellium approximation is too simple. We should probably think about a more careful calculation in a real system as producing two equivalent terms, which vary in approximately the same way with  $k_{TF}$  and  $\omega_q$ , but with prefactors which are arbitrary. In some ma-

terials, then, the second term might “win” at low frequencies, depending on details.

### 5.3 Cooper problem

A great deal was known about the phenomenology of superconductivity in the 1950’s, and it was already suspected that the electron phonon interaction was responsible, but the microscopic form of the wave function was unknown. A clue was provided by Leon Cooper, who showed that the noninteracting Fermi sea is *unstable* towards the addition of a single pair of electrons with attractive interactions. Cooper began by examining the wave function of this pair  $\psi(r_1, r_2)$ , which can always be written as a sum over plane waves

$$\psi(r_1, r_2) = \sum_{kq} u_k(q) e^{ik \cdot r_1} e^{-i(k+q) \cdot r_2} \zeta \quad (2)$$

where the  $u_k(q)$  are expansion coefficients and  $\zeta$  is the spin part of the wave function, either the singlet  $|\uparrow\downarrow - \downarrow\uparrow\rangle / \sqrt{2}$  or one of the triplet,  $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow + \downarrow\uparrow\rangle / \sqrt{2}$ . In fact since we will demand that  $\psi$  is the ground state of the two-electron system, we will assume the wave function is realized with zero center of mass momentum of the two electrons,  $u_k(q) = u_k \delta_{q,0}$ . Here is a quick argument related to the electron-phonon origin of the attractive interaction.<sup>1</sup> The electron-phonon interaction is strongest for those electrons with single-particle energies  $\xi_{\mathbf{k}}$  within  $\omega_D$  of the Fermi level. In the scattering process depicted in Fig. 3, momentum is

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<sup>1</sup>Thanks to Kevin McCarthy, who forced me to think about this further

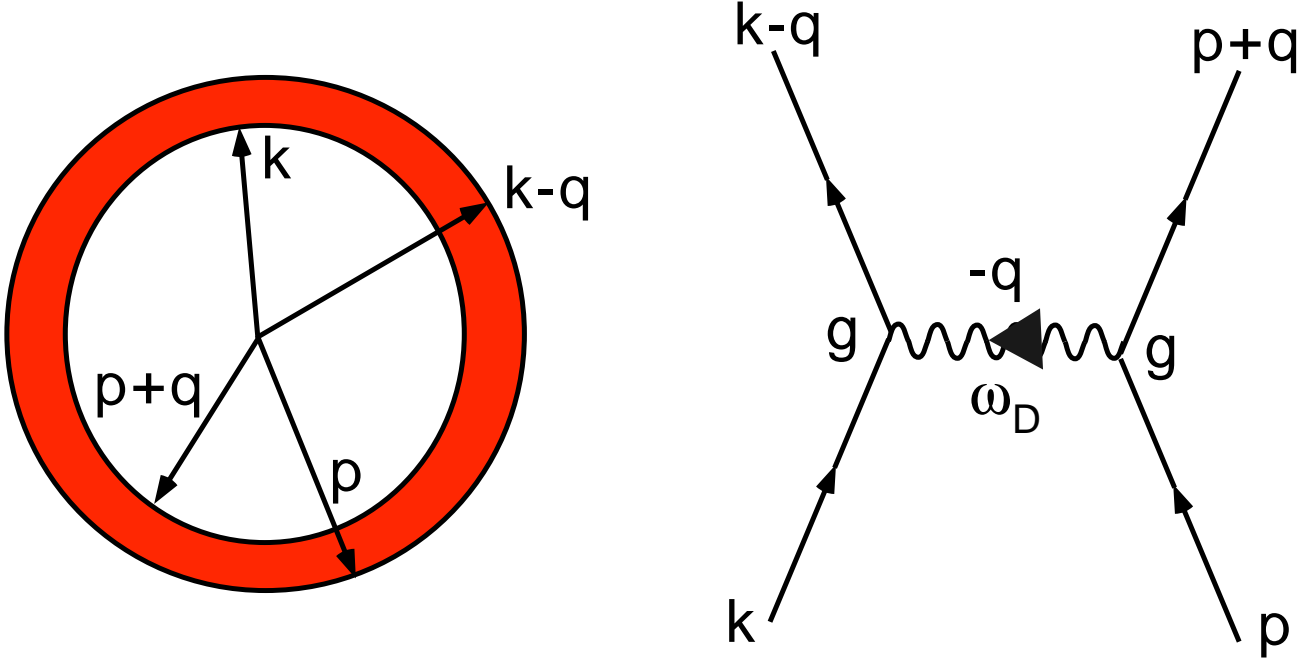


Figure 3: Electrons scattered by phonon exchange are confined to shell of thickness  $\omega_D$  about Fermi surface.

explicitly conserved, i.e. the total momentum

$$\mathbf{k} + \mathbf{p} = \mathbf{K} \quad (3)$$

is the same in the incoming and outgoing parts of the diagram. Now look at Figure 4, and note that if  $\mathbf{K}$  is not  $\sim 0$ , the phase space for scattering (attraction) is dramatically reduced. So the system can always lower its energy by creating  $\mathbf{K} = 0$  pairs. Henceforth we will make this assumption, as Cooper did.

Then  $\psi(r_1, r_2)$  becomes  $\sum_k u_k e^{ik \cdot (r_1 - r_2)}$ . Note that if  $u_k$  is *even* in  $k$ , the wave function has only terms  $\propto \cos k \cdot (r_1 - r_2)$ , whereas if it is *odd*, only the  $\sin k \cdot (r_1 - r_2)$  will contribute. This is an important distinction, because only in the former case is there an amplitude for the two electrons to live "on top of each other" at the origin. Note further that in order to

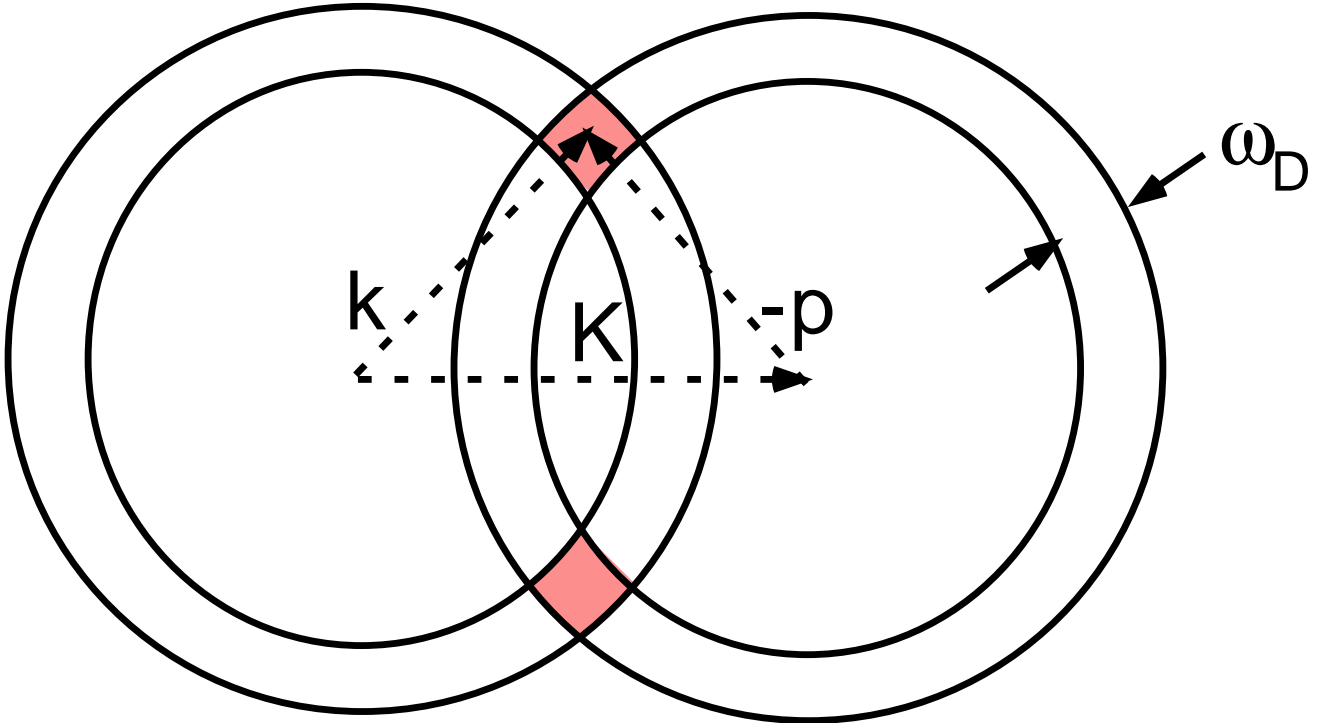


Figure 4: To get (attractive) scattering with finite cm momentum  $\mathbf{K}$ , need both electron energies to be within  $\omega_D$  of Fermi level– very little phase space.

preserve the proper overall antisymmetry of the wave function,  $u_k$  even (odd) in  $k$  implies the wave function must be spin singlet (triplet). Let us assume further that there is a general two-body interaction between the two electrons (the rest of the Fermi sea is noninteracting in the model!)  $V(r_1, r_2)$ , so that the Hamiltonian for the system is

$$H = -\frac{\nabla_1^2}{2m} - \frac{\nabla_2^2}{2m} + V(r_1, r_2). \quad (4)$$

Inserting the assumed form of  $\psi$  into the Schrödinger equation  $H\psi = E\psi$ , and Fourier transforming both sides with respect to the relative coordinate,  $r = r_1 - r_2$ , we find

$$(E - 2\epsilon_k)u_k = \sum_{k' > k_F} V_{kk'}u_{k'}, \quad (5)$$

where  $\epsilon_k = k^2/2m$  and the  $V_{kk'} = \int d^3r V(r)e^{i(k'-k)\cdot r}$  are the

matrix elements of the two-body interaction.

Recall  $k, k'$  correspond to energies at the Fermi level  $\epsilon_F$  in the absence of  $V$ . The question was posed by Cooper, is it possible to find an eigenvalue  $E < 2\epsilon_F$ , i.e. a *bound state* of the two electrons? To simplify the problem, Cooper assumed a model form for  $V_{kk'}$  in which

$$V_{kk'} = \begin{cases} -V & \xi_k, \xi_{k'} < \omega_c \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

where as usual  $\xi_k \equiv \epsilon_k - \epsilon_F$ . The BCS interaction is sometimes referred to as a “residual” attractive interaction, i.e. what is left when the long-range Coulomb interaction has been absorbed into renormalized electron-phonon coupling constants, etc., as in (1). The bound state equation becomes

$$u_k = \frac{V \sum'_{k'} u_{k'}}{2\epsilon_k - E}, \quad (7)$$

where the prime on the summation in this context means sum only over  $k$  such that  $\epsilon_f < \epsilon_k < \epsilon_F + \omega_c$ . Now  $u_k$  may be eliminated from the equation by summing both sides  $\sum_k$ , yielding

$$\frac{1}{V} = \sum'_k \frac{1}{2\epsilon_k - E} \quad (8)$$

$$\simeq \frac{1}{2} N_0 \int_{\epsilon_F}^{\epsilon_F + \omega_c} d\epsilon \frac{1}{2\epsilon - E} = \frac{1}{2} N_0 \log \frac{2\epsilon_F + 2\omega_c - E}{2\epsilon_F - E}. \quad (9)$$

For a weak interaction  $N_0 V \ll 1$ , we expect a solution (if at all) just below the Fermi level, so we treat  $2\epsilon_F - E$  as a small

positive quantity, e.g. negligible compared to  $2\omega_c$ . We then arrive at the pair binding energy

$$\Delta_{\text{Cooper}} \equiv 2\epsilon_F - E \simeq 2\omega_c e^{-2/N_0 V}. \quad (10)$$

There are several remarks to be made about this result.

1. Note (for your own information—Cooper didn't know this at the time!) that the dependence of the bound state energy on both the interaction  $V$  and the cutoff frequency  $\omega_c$  strongly resembles the famous BCS transition temperature dependence, with  $\omega_c$  identified as the phonon frequency  $\omega_D$ , as given in equation (I.1).
2. the dependence on  $V$  is that of an essential singularity, i.e. a nonanalytic function of the parameter. Thus we may expect never to arrive at this result at any order in perturbation theory, an unexpected problem which hindered theoretical progress for a long time.
3. The solution found has isotropic or s-symmetry, since it doesn't depend on the  $\hat{k}$  on the Fermi surface. (How would an angular dependence arise? Look back over the calculation.)
4. Note the integrand  $(2\epsilon_k - E)^{-1} = (2\xi_k + \Delta_{\text{Cooper}})^{-1}$  peaks at the Fermi level with energy spread  $\Delta_{\text{Cooper}}$  of states involved in the pairing. The weak-coupling ( $N_0 V \ll 1$ ) solution therefore provides a bit of *a posteriori* justification for its own existence, since the fact that  $\Delta_{\text{Cooper}} \ll \omega_c$  implies that the dependence of  $V_{kk'}$  on energies out near

the cutoff and beyond is in fact not terribly important, so the cutoff procedure used was ok.

5. The spread in momentum is therefore roughly  $\Delta_{\text{Cooper}}/v_F$ , and the characteristic size of the pair (using Heisenberg's uncertainty relation) about  $v_F/T_c$ . This is about 100-1000Å in metals, so since there is of order 1 electron/ unit cell in a metal, and if this toy calculation has anything to do with superconductivity, there are certainly many electron pairs overlapping each other in real space in a superconductor.

#### 5.4 Pair condensate & BCS Wavefctn.

Obviously one thing is missing from Cooper's picture: if it is energetically favorable for two electrons in the presence of a noninteracting Fermi sea to *pair*, i.e. to form a bound state, why not have the other electrons pair too, and lower the energy of the system still further? This is an *instability* of the normal state, just like magnetism or charge density wave formation, where a ground state of completely different character (and symmetry) than the Fermi liquid is stabilized. The Cooper calculation is a T=0 problem, but we expect that as one lowers the temperature, it will become at some critical temperature  $T_c$  energetically favorable for *all* the electrons to pair. Although this picture is appealing, many things about it are unclear: does the pairing of many other electrons alter the attractive interaction which led to the pairing in the first

place? Does the bound state energy per pair change? Do all of the electrons in the Fermi sea participate? And most importantly, how does the critical temperature actually depend on the parameters and can we calculate it?

## 5.5 BCS Model.

A consistent theory of superconductivity may be constructed either using the full “effective interaction” or our approximation  $V(\mathbf{q}, \omega)$  to it. However almost all interesting questions can be answered by the even simpler model used by BCS. The essential point is to have an attractive interaction for electrons in a shell near the Fermi surface; retardation is secondary. Therefore BCS proposed starting from a phenomenological Hamiltonian describing free electrons scattering via an effective instantaneous interaction à la Cooper:

$$H = H_0 - V \sum_{\substack{kk'q \\ \sigma\sigma'}}' c_{k\sigma}^\dagger c_{-k+q\sigma'}^\dagger c_{-k'+q\sigma'} c_{k'\sigma}, \quad (11)$$

where the prime on the sum indicates that the energies of the states  $k$  and  $k'$  must lie in the shell of thickness  $\omega_D$ . Note the interaction term is just the Fourier transform of a completely *local* 4-Fermi interaction  $\psi^\dagger(r)\psi^\dagger(r)\psi(r)\psi(r)$ .<sup>2</sup>

Recall that in our discussion of the instability of the normal state, we suggested that an infinitesimal pair field could produce a finite amplitude for pairing. That amplitude was the expectation value  $\langle c_{k\sigma}^\dagger c_{-k-\sigma}^\dagger \rangle$ . We ignore for the moment

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<sup>2</sup>Note this is not the most general form leading to superconductivity. Pairing in higher angular momentum channels requires a *bilocal* model Hamiltonian, as we shall see later.



the problems with number conservation, and ask if we can simplify the Hamiltonian still further with a mean field approximation, again to be justified *a posteriori*. We proceed along the lines of generalized Hartree-Fock theory, and rewrite the interaction as

$$c_{k\sigma}^\dagger c_{-k+q\sigma'}^\dagger c_{-k'+q\sigma'} c_{k'\sigma} = [\langle c_{k\sigma}^\dagger c_{-k+q\sigma'}^\dagger \rangle + \delta(c^\dagger c^\dagger)] \times \\ \times [\langle c_{-k'+q\sigma'} c_{k'\sigma} \rangle + \delta(cc)], \quad (12)$$

where, e.g.  $\delta(cc) = c_{-k'+q\sigma'} c_{k'\sigma} - \langle c_{-k'+q\sigma'} c_{k'\sigma} \rangle$  is the *fluctuation* of this operator about its expectation value. If a mean field description is to be valid, we should be able to neglect terms quadratic in the fluctuations when we expand Eq (20). If we furthermore make the assumption that pairing will take place in a uniform state (zero pair center of mass momentum), then we put  $\langle c_{-k'+q\sigma'} c_{k'\sigma} \rangle = \langle c_{-k'\sigma'} c_{k'\sigma} \rangle \delta_{q,0}$ . The effective Hamiltonian then becomes (check!)

$$H \simeq H_0 - (\Delta \sum_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c.) + \Delta_k \langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \rangle^*, \quad (13)$$

where

$$\Delta = V \sum_k \langle c_{-k\downarrow} c_{k\uparrow} \rangle. \quad (14)$$

What BCS (actually Bogoliubov, after BCS) did was then to treat the *order parameter*  $\Delta$  as a (complex) number, and calculate expectation values in the approximate Hamiltonian (13), insisting that  $\Delta$  be determined self-consistently via Eq. (14) at the same time.

### 5.5.1 BCS wave function, gauge invariance, and number conservation.

What BCS actually did in their original paper is to treat the Hamiltonian (11) variationally. Their ansatz for the ground state of (11) is a trial state with the pairs  $k \uparrow, -k \downarrow$  occupied with amplitude  $v_k$  and unoccupied with amplitude  $u_k$ , such that  $|u_k|^2 + |v_k|^2 = 1$ :

$$|\psi \rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0 \rangle. \quad (15)$$

This is a *variational* wave function, so the energy is to be minimized over the space of  $u_k, v_k$ . Alternatively, one can diagonalize the Hartree-Fock (BCS) Hamiltonian directly, together with the self-consistency equation for the order parameter; the two methods turn out to be equivalent. I will follow the latter procedure, but first make a few remarks on the form of the wave function. First, note the explicit violation of particle number conservation:  $|\psi \rangle$  is a superposition of states describing 0, 2, 4, ..., N-particle systems.<sup>3</sup> In general a quantum mechanical system with fixed particle number  $N$  (like, e.g. a real superconductor!) manifests a global  $U(1)$  gauge symmetry, because  $H$  is invariant under  $c_{k\sigma}^\dagger \rightarrow e^{i\theta} c_{k\sigma}^\dagger$ . The state  $|\psi \rangle$  is characterized by a set of coefficients  $\{u_k, v_k\}$ , which becomes  $\{u_k, e^{2i\theta} v_k\}$  after the gauge transformation. The two states  $|\psi \rangle$  and  $|\psi(\phi)\rangle$ , where  $\phi = 2\theta$ , are inequivalent, mutually orthogonal quantum states, since they are not

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<sup>3</sup>What happened to the odd numbers? In mesoscopic superconductors, there are actually differences in the properties of even and odd-number particle systems, but for bulk systems the distinction is irrelevant.

simply related by a multiplicative phase factor.<sup>4</sup> Since  $H$  is independent of  $\phi$ , however, all states  $|\psi(\phi)\rangle$  are continuously degenerate, i.e. the ground state has a  $U(1)$  gauge (phase) symmetry. Any state  $|\psi(\phi)\rangle$  is said to be a broken symmetry state, because it is not invariant under a  $U(1)$  transformation, i.e. the system has "chosen" a particular  $\phi$  out of the degenerate range  $0 < \phi < 2\pi$ . Nevertheless the absolute value of the overall phase of the ground state is not an observable, but its variations  $\delta\phi(r, t)$  in space and time are. It is the *rigidity* of the phase, i.e. the energy cost of any of these fluctuations, which is responsible for superconductivity.

Earlier I mentioned that it was possible to construct a number conserving theory. It is now instructive to see how: states of definite number are formed [Anderson 1958] by making coherent superpositions of states of definite phase

$$|\psi(N)\rangle = \int_0^{2\pi} d\phi e^{i\phi N/2} |\psi(\phi)\rangle. \quad (16)$$

[The integration over  $\phi$  gives zero unless there are in the expansion of the product contained in  $|\psi\rangle$  precisely  $N/2$  pair creation terms, each with factor  $\exp i\phi$ .] Note while this state has maximal uncertainty in the *value* of the phase, the rigidity of the system to phase fluctuations is retained.<sup>5</sup>

It is now straightforward to see why BCS theory works. The BCS wave function  $|\psi\rangle$  may be expressed as a sum  $|\psi\rangle = \sum_N a_N |\psi(N)\rangle$  [Convince yourself of this by calculat-

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<sup>4</sup>In the normal state,  $|\psi\rangle$  and  $\psi(\phi)$  differ by a global multiplicative phase  $e^{i\theta}$ , which has no physical consequences, and the ground state is nondegenerate.

<sup>5</sup>The phase and number are in fact canonically conjugate variables,  $[N/2, \phi] = i$ , where  $N = 2i\partial/\partial\phi$  in the  $\phi$  representation.

ing the  $a_N$  explicitly!]. IF we can show that the distribution of coefficients  $a_N$  is sharply peaked about its mean value  $\langle N \rangle$ , then we will get essentially the same answers as working with a state of definite number  $N = \langle N \rangle$ . Using the explicit form (23), it is easy to show

$$\langle N \rangle = \langle \psi | \sum_{k\sigma} n_{k\sigma} | \psi \rangle = 2 \sum_k |v_k|^2 \quad ; \quad \langle (N - \langle N \rangle)^2 \rangle = \sum_k u_k^2 v_k^2. \quad (17)$$

Now the  $u_k$  and  $v_k$  will typically be numbers of order 1, so since the numbers of allowed  $k$ -states appearing in the  $k$  sums scale with the volume of the system, we have  $\langle N \rangle \sim V$ , and  $\langle (N - \langle N \rangle)^2 \rangle \sim V$ . Therefore the *width* of the distribution of numbers in the BCS state is  $\langle (N - \langle N \rangle)^2 \rangle^{1/2} / \langle N \rangle \sim N^{-1/2}$ . As  $N \rightarrow 10^{23}$  particles, this relative error implied by the number nonconservation in the BCS state becomes negligible.

### 5.5.2 Is the BCS order parameter general?

Before leaving the subject of the phase in this section, it is worthwhile asking again why we decided to pair states with opposite momenta and spin,  $k \uparrow$  and  $-k \downarrow$ . The BCS argument had to do 1) with minimizing the energy of the entire system by giving the Cooper pairs zero center of mass momentum, and 2) insisting on a spin singlet state because the phonon mechanism leads to electron attraction when the electrons are at the same spatial position (because it is retarded in time!), and a spatially symmetric wavefunction with large

amplitude at the origin demands an antisymmetric spin part. Can we relax these assumptions at all? The first requirement seems fairly general, but it should be recalled that one can couple to the pair center of mass with an external magnetic field, so that one will create spatially inhomogeneous (finite- $q$ ) states with current flow in the presence of a magnetic field. Even in zero external field, it has been proposed that systems with coexisting antiferromagnetic correlations could have pairing with finite antiferromagnetic nesting vector  $\vec{Q}$  [Baltensberger and Strässler 196?]. The requirement for singlet pairing can clearly be relaxed if there is a pairing mechanism which disfavors close approach of the paired particles. This is the case in superfluid  $^3\text{He}$ , where the hard core repulsion of two  $^3\text{He}$  atoms suppresses  $T_c$  for s-wave, singlet pairing and enhances  $T_c$  for p-wave, triplet pairing where the amplitude for two particles to be together at the origin is always zero.

In general, pairing is possible for some pair mechanism if the single particle energies corresponding to the states  $k\sigma$  and  $k'\sigma'$  are degenerate, since in this case the pairing interaction is most attractive. In the BCS case, a guarantee of this degeneracy for  $k \uparrow$  and  $-k \downarrow$  in zero field is provided by Kramer's theorem, which says these states must be degenerate because they are connected by *time reversal* symmetry. However, there are other symmetries: in a system with inversion symmetry, *parity* will provide another type of degeneracy, so  $k \uparrow$ ,  $k \downarrow$ ,  $-k \uparrow$  and  $-k \downarrow$  are all degenerate and may be paired

with one another if allowed by the pair interaction.

## 5.6 Thermodynamics

### 5.6.1 Bogoliubov transformation

We now return to (13) and discuss the solution by canonical transformation given by Bogoliubov. After our drastic approximation, we are left with a quadratic Hamiltonian in the  $c$ 's, but with  $c^\dagger c^\dagger$  and  $cc$  terms in addition to  $c^\dagger c$ 's. We can diagonalize it easily, however, by introducing the *quasiparticle operators*  $\gamma_{\mathbf{k}0}$  and  $\gamma_{\mathbf{k}1}$  by

$$\begin{aligned} c_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}^* \gamma_{\mathbf{k}0} + v_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger \\ c_{-\mathbf{k}\downarrow}^\dagger &= -v_{\mathbf{k}}^* \gamma_{\mathbf{k}0} + u_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger. \end{aligned} \quad (18)$$

You may check that this transformation is canonical (preserves fermion comm. rels.) if  $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ . Substituting into (13) and using the commutation relations we get

$$\begin{aligned} H_{BCS} &= \sum_{\mathbf{k}} \xi_{\mathbf{k}} [ (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) (\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} + \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1}) + 2|v_{\mathbf{k}}|^2 \\ &\quad + 2u_{\mathbf{k}}^* v_{\mathbf{k}}^* \gamma_{\mathbf{k}1} \gamma_{\mathbf{k}0} + 2u_{\mathbf{k}} v_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}0}^\dagger ] \\ &\quad + \sum_{\mathbf{k}} [ (\Delta_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}^* + \Delta_{\mathbf{k}}^* u_{\mathbf{k}}^* v_{\mathbf{k}}) (\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} + \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1} - 1) \\ &\quad + (\Delta_{\mathbf{k}} v_{\mathbf{k}}^{*2} - \Delta_{\mathbf{k}}^* u_{\mathbf{k}}^{*2}) \gamma_{\mathbf{k}1} \gamma_{\mathbf{k}0} + (\Delta_{\mathbf{k}}^* v_{\mathbf{k}}^2 - \Delta_{\mathbf{k}} u_{\mathbf{k}}^2) \gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}1}^\dagger \\ &\quad + \Delta_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \rangle^* ], \end{aligned} \quad (19)$$

which does not seem to be enormous progress, to say the least. But the game is to eliminate the terms which are not of the form  $\gamma^\dagger \gamma$ , so to be left with a sum of independent number-type

terms whose eigenvalues we can write down. The coefficients of the  $\gamma^\dagger\gamma^\dagger$  and  $\gamma\gamma$  type terms are seen to vanish if we choose

$$2\xi_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} + \Delta_{\mathbf{k}}^*v_{\mathbf{k}}^2 - \Delta_{\mathbf{k}}u_{\mathbf{k}}^2 = 0. \quad (20)$$

This condition and the normalization condition  $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$  are both satisfied by the solutions

$$\frac{|u_{\mathbf{k}}|^2}{|v_{\mathbf{k}}|^2} = \frac{1}{2} \left( 1 \pm \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad (21)$$

where I defined the *Bogolibov quasiparticle energy*

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}. \quad (22)$$

The BCS Hamiltonian has now been *diagonalized*:

$$H_{BCS} = \sum_{\mathbf{k}} E_{\mathbf{k}} \left( \gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} + \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1} \right) + \sum_{\mathbf{k}} \left( \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \rangle^* \right). \quad (23)$$

Note the second term is just a constant, which will be important for calculating the ground state energy accurately. The first term, however, just describes a set of *free fermion* excitations above the ground state, with spectrum  $E_{\mathbf{k}}$ .

### 5.6.2 Density of states

The BCS spectrum is easily seen to have a minimum  $\Delta_{\mathbf{k}}$  for a given direction  $\mathbf{k}$  on the Fermi surface;  $\Delta_{\mathbf{k}}$  therefore, in addition to playing the role of *order parameter* for the superconducting transition, is also the *energy gap* in the 1-particle spectrum. To see this explicitly, we can simply do

a change of variables in all energy integrals from the normal metal eigenenergies  $\xi_{\mathbf{k}}$  to the quasiparticle energies  $E_{\mathbf{k}}$ :

$$N(E)dE = N_N(\xi)d\xi. \quad (24)$$

If we are interested in the standard case where the gap  $\Delta$  is much smaller than the energy over which the normal state dos  $N_N(\xi)$  varies near the Fermi level, we can make the replacement

$$N_N(\xi) \simeq N_N(0) \equiv N_0, \quad (25)$$

so using the form of  $E_{\mathbf{k}}$  from (22) we find

$$\frac{N(E)}{N_0} = \begin{cases} \frac{E}{\sqrt{E^2 - \Delta^2}} & E > \Delta \\ 0 & E < \Delta \end{cases}. \quad (26)$$

This function is sketched in Figure 5.

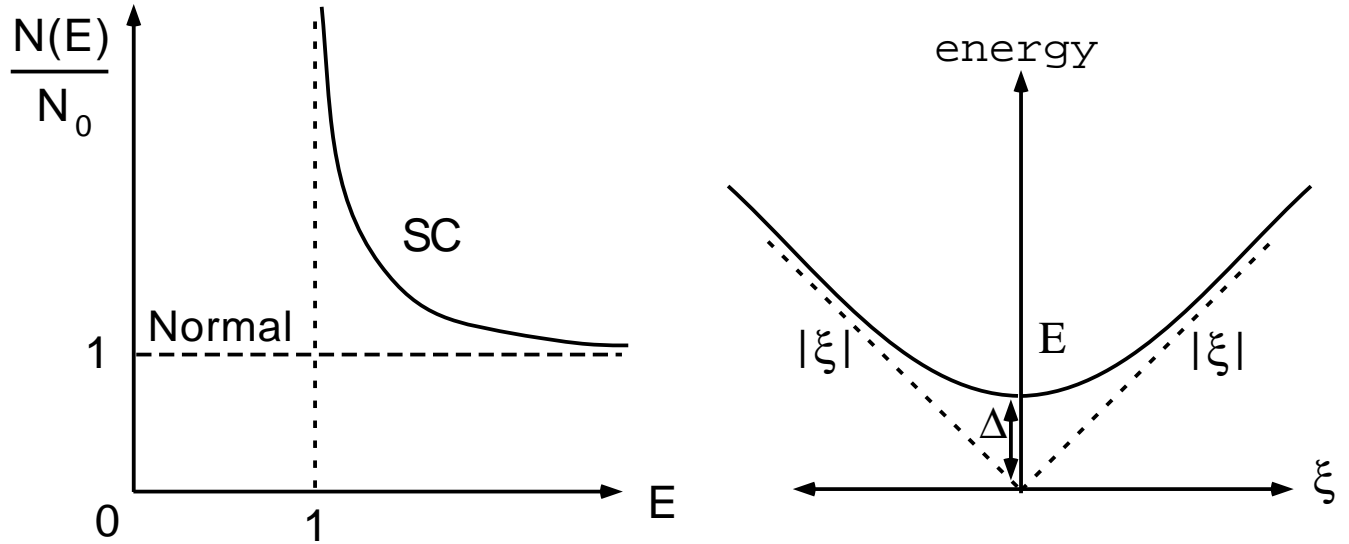


Figure 5: a) Normalized density of states; b) Quasiparticle spectrum.



### 5.6.3 Critical temperature

The critical temperature is defined as the temperature at which the order parameter  $\Delta_{\mathbf{k}}$  vanishes. We can now calculate this with the aid of the diagonalized Hamiltonian. The self-consistency condition is

$$\begin{aligned}\Delta_{\mathbf{k}}^* &= V \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger \rangle^* \\ &= V \sum_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}^* \langle 1 - \gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} - \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1} \rangle \\ &= V \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}^*}{2E_{\mathbf{k}}} (1 - 2f(E_{\mathbf{k}})).\end{aligned}\tag{27}$$

Since  $1 - 2f(E) = \tanh[E/(2T)]$ , the *BCS gap equation* reads

$$\Delta_{\mathbf{k}}^* = V \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}} \tanh \frac{E_{\mathbf{k}'}}{2T}\tag{28}$$

This equation may now be solved, first for the critical temperature itself, i.e. the temperature at which  $\Delta \rightarrow 0$ , and then for the normalized order parameter  $\Delta/T_c$  for any temperature  $T$ . It is the ability to eliminate all normal state parameters from the equation in favor of  $T_c$  itself which makes the BCS theory powerful. For in practice the parameters  $\omega_D$ ,  $N_0$ , and particularly  $V$  are known quite poorly, and the fact that two of them occur in an exponential makes an accurate first principles calculation of  $T_c$  nearly impossible. You should always be suspicious of a theory which claims to be able to calculate  $T_c$ ! On the other hand,  $T_c$  is easy to measure, so if it is the only energy scale in the theory, we have a tool with enormous predictive power.

First note that at  $T_c$ , the gap equation becomes

$$\frac{1}{N_0 V} = \int_0^{\omega_D} d\xi_k \frac{1}{\xi_k} \tanh \frac{\xi_k}{2T_c}. \quad (29)$$

This integral can be approximated carefully, but it is useful to get a sense of what is going on by doing a crude treatment. Note that since  $T_c \ll \omega_D$  generally, most of the integrand weight occurs for  $\xi > T$ , so we can estimate the tanh factor by 1. The integral is log divergent, which is why the cutoff  $\omega_D$  is so important. We find

$$\frac{1}{N_0 V_0} = \log \frac{\omega}{T_c} \Rightarrow T_c \simeq \omega_D e^{-1/N_0 V} \quad (30)$$

The more accurate analysis of the integral gives the BCS result

$$\boxed{T_c = 1.14 \omega_D e^{-1/N_0 V}} \quad (31)$$

We can do the same calculation *near*  $T_c$ , expanding to leading order in the small quantity  $\Delta(T)/T$ , to find  $\Delta(T)/T_c \simeq 3.06(1 - T/T_c)^{1/2}$ . At  $T = 0$  we have

$$\frac{1}{N_0 V} = \int_0^{\omega_D} d\xi_k \frac{1}{E_k} = \int_{\Delta}^{\omega_D} dE N(E)/E \quad (32)$$

$$= \int_{\Delta}^{\omega_D} dE \frac{1}{\sqrt{E^2 - \Delta^2}} \simeq \ln(2\omega_d/\Delta), \quad (33)$$

so that  $\Delta(0) \simeq 2\omega_D \exp -1/N_0 V$ , or  $\Delta(0)/T_c \simeq 1.76$ . The full temperature dependence of  $\Delta(T)$  is sketched in Figure 6). In the halcyon days of superconductivity theory, comparisons with the theory had to be compared with a careful table of  $\Delta/T_c$  painstakingly calculated and compiled by Mühlischlegl.

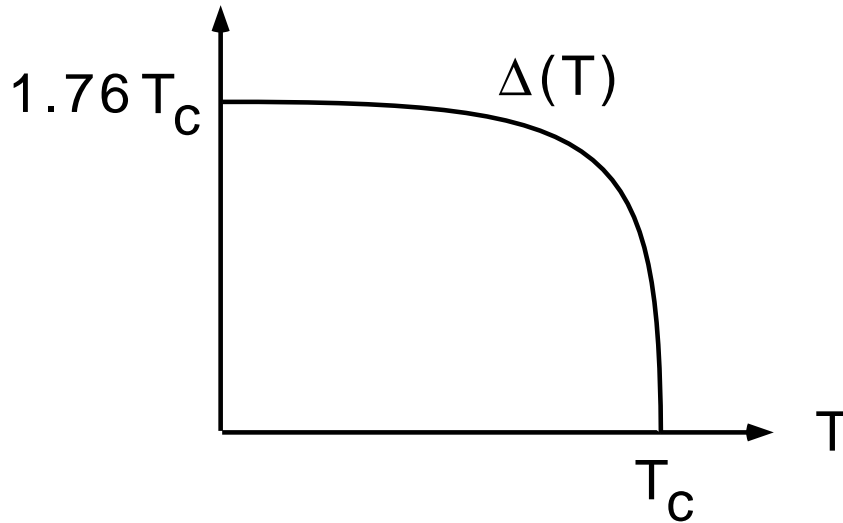


Figure 6: BCS order parameter as fctn. of  $T$ .

Nowadays the numerical solution requires a few seconds on a PC. It is frequently even easier to use a phenomenological approximate closed form of the gap, which is correct near  $T = 0$  and  $T = T_c$ :

$$\Delta(T) = \delta_{sc} T_c \tanh\left\{\frac{\pi}{\delta_{sc}} \sqrt{a \frac{\delta C}{C_N} \left(\frac{T_c}{T} - 1\right)}\right\}, \quad (34)$$

where  $\delta_{sc} = \Delta(0)/T_c = 1.76$ ,  $a = 2/3$ , and  $\delta C/C_N = 1.43$  is the normalized specific heat jump.<sup>6</sup> This is another of the “universal” ratios which the BCS theory predicted and which helped confirm the theory in classic superconductors.

#### 5.6.4 Specific heat.

The gap in the density of states is reflected in all thermodynamic quantities as an activated behavior  $e^{-\Delta/T}$ , at low  $T$ , due to the exponentially small number of Bogoliubov quasi-

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<sup>6</sup>Note to evaluate the last quantity, we need only use the calculated temperature dependence of  $\Delta$  near  $T_c$ , and insert into Eq. (47).

particles with thermal energy sufficient to be excited over the gap  $\Delta$  at low temperatures  $T \ll \Delta$ . The electronic specific heat is particularly easy to calculate, since the entropy of the BCS superconductor is once again the entropy of a *free* gas of noninteracting quasiparticles, with modified spectrum  $E_k$ . The expression (II.6) then gives the entropy directly, and may be rewritten

$$S = -k_B \int_0^\infty dE N(E) \{ f(E) \ln f(E) + [1 - f(E)] \ln [1 - f(E)] \}, \quad (35)$$

where  $f(E)$  is the Fermi function. The constant volume specific heat is just  $C_{el,V} = T[dS/dT]_V$ , which after a little algebra may be written

$$C_{el,V} = \frac{2}{T} \int dE N(E) \left( \frac{-\partial f}{\partial E} \right) \left[ E^2 - \frac{1}{2} T \frac{d\Delta^2}{dT} \right]. \quad (36)$$

A sketch of the result of a full numerical evaluation is shown in Figure 1. Note the discontinuity at  $T_c$  and the very rapid falloff at low temperatures.

It is instructive to actually calculate the entropy and specific heat both at low temperatures and near  $T_c$ . For  $T \ll \Delta$ ,  $f(E) \simeq e^{-E/T}$  and the density of states factor  $N(E)$  in the integral cuts off the integration at the lower limit  $\Delta$ , giving  $C \simeq (N_0 \Delta^{5/2} / T^{3/2}) e^{-\Delta/T}$ .<sup>7</sup>

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<sup>7</sup>To obtain this, try the following:

- replace the derivative of Fermi function by  $\exp(-E/T)$
- do integral by parts to remove singularity at  $\Delta$
- expand around  $\Delta$   $E = \Delta + \delta E$
- change integration variables from  $E$  to  $\delta E$

Somebody please check my answer!

Note the first term in Eq. (47) is continuous through the transition  $\Delta \rightarrow 0$  (and reduces to the normal state specific heat  $(2\pi^2/3)N_0T$  above  $T_c$ ), but the second one gives a discontinuity at  $T_c$  of  $(C_N - C_S)/C_N = 1.43$ , where  $C_S = C(T_c^-)$  and  $C_N = C(T_c^+)$ . To evaluate (36), we need the T dependence of the order parameter from a general solution of (28).

## 5.7 Electrodynamics

### 5.7.1 Linear response to vector potential

The existence of an energy gap is not a sufficient condition for superconductivity (actually, it is not even a necessary one!). Insulators, for example, do not possess the *phase rigidity* which leads to perfect conductivity and perfect diamagnetism which are the defining characteristics of superconductivity. We can understand both properties by calculating the current response of the system to an applied magnetic or electric field. The kinetic energy in the presence of an applied vector potential  $\mathbf{A}$  is just

$$H_0 = \frac{1}{2m} \sum_{\sigma} \int d^3r \psi_{\sigma}^{\dagger}(r) [-i\nabla - (\frac{e}{c})\mathbf{A}]^2 \psi_{\sigma}(r), \quad (37)$$

and the second quantized current density operator is given by

$$\mathbf{j}(r) = \frac{e}{2m} \{ \psi^{\dagger}(r) (-i\nabla - \frac{e}{c}\mathbf{A}) \psi(r) + [(i\nabla - \frac{e}{c}\mathbf{A}) \psi^{\dagger}(r)] \psi(r) \} \quad (38)$$

$$= \mathbf{j}_{para} - \frac{e^2}{mc} \psi^{\dagger}(r) \psi(r) \mathbf{A}, \quad (39)$$

where

$$\mathbf{j}_{para}(r) = \frac{-ie}{2m} \{ \psi^\dagger(r) \nabla \psi(r) - (\nabla \psi^\dagger(r)) \psi(r) \}, \quad (40)$$

or in Fourier space,

$$\mathbf{j}_{para}(\mathbf{q}) = \frac{e}{m} \sum_{\mathbf{k}\sigma} \mathbf{k} c_{\mathbf{k}-\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (41)$$

We would like to do a calculation of the linear current response  $\mathbf{j}(q, \omega)$  to the application of an external field  $\mathbf{A}(q, \omega)$  to the system a long time after the perturbation is turned on. Expanding the Hamiltonian to first order in  $\mathbf{A}$  gives the interaction

$$H' = \int d^3r \mathbf{j}_{para} \cdot \mathbf{A} = \frac{e}{mc} \sum_{\mathbf{k}\sigma} \mathbf{k} \cdot \mathbf{A}(\mathbf{q}) c_{\mathbf{k}-\mathbf{q}\sigma}^\dagger c_{\mathbf{q}\sigma}. \quad (42)$$

The expectation value  $\langle \mathbf{j} \rangle$  may now be calculated to linear order via the Kubo formula, yielding

$$\langle \mathbf{j} \rangle(\mathbf{q}, \omega) = \underline{K}(\mathbf{q}, \omega) \mathbf{A}(\mathbf{q}, \omega) \quad (43)$$

with

$$\underline{K}(\mathbf{q}, \omega) = -\frac{ne^2}{mc} + \langle [\mathbf{j}_{para}, \mathbf{j}_{para}] \rangle(\mathbf{q}, \omega). \quad (44)$$

Note the first term in the current

$$\mathbf{j}_{dia}(\mathbf{q}, \omega) \equiv -\frac{ne^2}{mc} \mathbf{A}(\mathbf{q}, \omega) \quad (45)$$

is purely *diamagnetic*, i.e. these currents tend to screen the external field (note sign). The second, *paramagnetic* term is formally the Fourier transform of the current-current correlation function (correlation function used in the sense of our

discussion of the Kubo formula).<sup>8</sup> Here are a few remarks on this expression:

- Note the simple product structure of (43) in momentum space implies a *nonlocal* relationship in general between  $\mathbf{j}$  and  $\mathbf{A}$ , i.e.  $\mathbf{j}(r)$  depends on the  $\mathbf{A}(r')$  at many points  $r'$  around  $r$ .<sup>9</sup>
- Note also that the electric field in a gauge where the electrostatic potential is set to zero may be written  $\mathbf{E}(\mathbf{q}, \omega) = -i\omega\mathbf{A}(\mathbf{q}, \omega)$ , so that the *complex* conductivity of the system defined by  $\mathbf{j} = \underline{\sigma}\mathbf{E}$  may be written

$$\underline{\sigma}(\mathbf{q}, \omega) = \frac{i}{\omega} \underline{K}(\mathbf{q}, \omega) \quad (47)$$

- What happens in a normal metal? The paramagnetic second term *cancels* the diamagnetic response at  $\omega = 0$ , leaving no real part of  $K$  (Im part of  $\sigma$ ), i.e. the conductivity is purely dissipative and not inductive at  $\omega, \mathbf{q} = 0$  in the normal metal.

### 5.7.2 Meissner Effect.

There is a theorem of classical physics proved by Bohr<sup>10</sup> which states that the ground state of a system of charged particles

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<sup>8</sup>We will see that the first term gives the *diamagnetic* response of the system, and the second the temperature-dependent *paramagnetic* response.

<sup>9</sup>If we transformed back, we'd get the convolution

$$\mathbf{j}(\mathbf{r}) = \int d^3r' K(\mathbf{r}, \mathbf{r}') \mathbf{A}(\mathbf{r}') \quad (46)$$

<sup>10</sup>See “The development of the quantum-mechanical electron theory of metals: 1928-33.” L. Hoddeson and G. Baym, Rev. Mod. Phys., 59, 287 (1987).

in an external magnetic field carries zero current. The essential element in the proof of this theorem is the fact that the magnetic forces on the particles are always perpendicular to their velocities. In a quantum mechanical system, the three components of the velocity do not commute in the presence of the field, allowing for a finite current to be created in the ground state. Thus the existence of the Meissner effect in superconductors, wherein magnetic flux is expelled from the interior of a sample below its critical temperature, is a clear proof that superconductivity is a manifestation of quantum mechanics.

The typical theorists' geometry for calculating the penetration of an electromagnetic field into a superconductor is the half-space shown in Figure 7, and compared to schematics of practical experimental setups involving resonant coils and microwave cavities in Figs. 7 a)-c). In the *gedanken* experiment

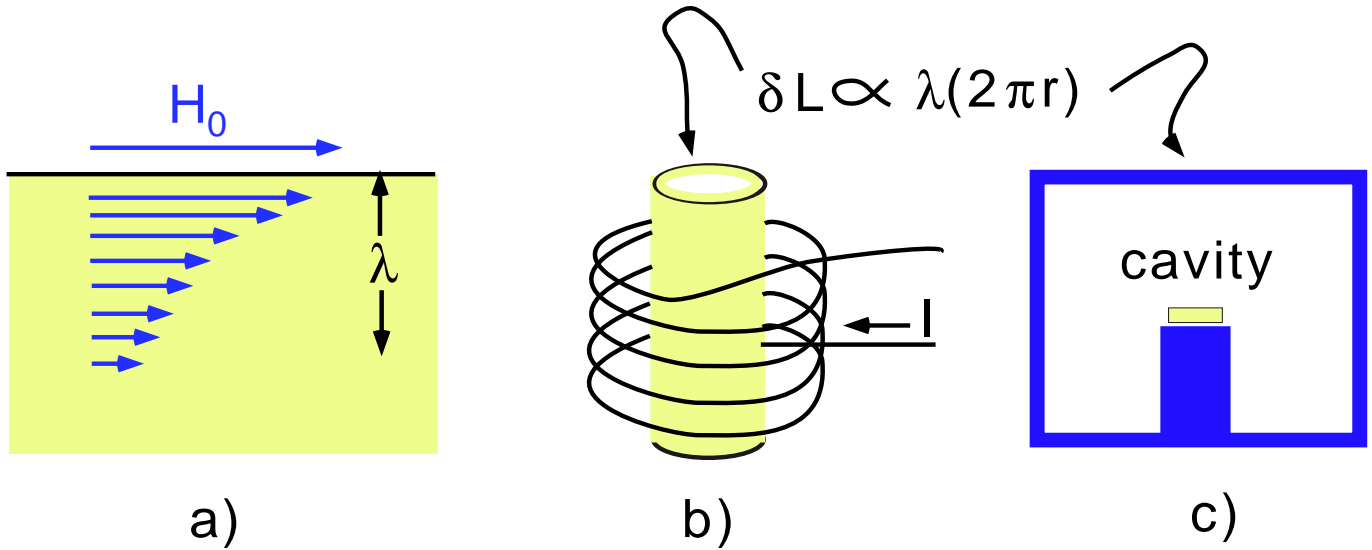


Figure 7: a) Half-space geometry for penetration depth calculation; b) Resonant coil setup; c) Microwave cavity



case, a DC field is applied parallel to the sample surface, and currents and fields are therefore functions only of the coordinate perpendicular to the surface,  $\mathbf{A} = \mathbf{A}(z)$ , etc. Since we are interested in an external electromagnetic wave of very long wavelength compared to the sample size, and zero frequency, we need the limit  $\omega = 0, q \rightarrow \infty$  of the response. We will assume that in this limit  $\underline{K}(0, 0) \rightarrow \text{const}$ , which we will call  $-(c/4\pi)\lambda^{-2}$  for reasons which will become clear! Equation (63) then has the form

$$\mathbf{j} = -\frac{c}{4\pi}\lambda^{-2}\mathbf{A}, \quad (48)$$

This is sometimes called London's equation, which must be solved in conjunction with Maxwell's equation

$$\nabla \times \mathbf{B} = -\nabla^2 \mathbf{A} = \frac{4\pi}{c}\mathbf{j} = -\lambda^{-2}\mathbf{A}, \quad (49)$$

which immediately gives  $\mathbf{A} \sim e^{-z/\lambda}$ , and  $\mathbf{B} = \mathbf{B}_0 e^{-z/\lambda}$ . The currents evidently screen the fields for distances below the surface greater than about  $\lambda$ . This is precisely the Meissner effect, which therefore follows *only* from our assumption that  $K(0, 0) = \text{const}$ . A BCS calculation will now tell us how the “penetration depth”  $\lambda$  depends on temperature.

Evaluating the expressions in (44) in full generality is tedious and is usually done with standard many-body methods beyond the scope of this course. However for  $\mathbf{q} = 0$  the calculation is simple enough to do without resorting to Green's functions. First note that the perturbing Hamiltonian  $H'$  may

be written in terms of the quasiparticle operators (18) as

$$H' = \quad (50)$$

$$\begin{aligned} & -\frac{e}{mc} \sum_{\mathbf{k}} \mathbf{k} \cdot \mathbf{A}(\mathbf{q}) \left[ (u_{\mathbf{k}} u_{\mathbf{k}+\mathbf{q}} + v_{\mathbf{k}} v_{\mathbf{k}+\mathbf{q}}) (\gamma_{\mathbf{k}+\mathbf{q}0}^\dagger \gamma_{\mathbf{k}0} - \gamma_{\mathbf{k}+\mathbf{q}1}^\dagger \gamma_{\mathbf{k}1}) \right. \\ & \left. + (v_{\mathbf{k}} u_{\mathbf{k}+\mathbf{q}} - u_{\mathbf{k}} v_{\mathbf{k}+\mathbf{q}}) (\gamma_{\mathbf{k}+\mathbf{q}0}^\dagger \gamma_{\mathbf{k}1}^\dagger - \gamma_{\mathbf{k}+\mathbf{q}1} \gamma_{\mathbf{k}0}) \right] \\ & \xrightarrow{q \rightarrow 0} -\frac{e}{mc} \sum_{\mathbf{k}} \mathbf{k} \cdot \mathbf{A}(0) (\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} - \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1}) \end{aligned} \quad (51)$$

If you compare with the  $\mathbf{A} = \mathbf{0}$  Hamiltonian (23), we see that the new excitations of the system are

$$\begin{aligned} E_{\mathbf{k}0} & \rightarrow E_{\mathbf{k}} - \frac{e}{mc} \mathbf{k} \cdot \mathbf{A}(0) \\ E_{\mathbf{k}1} & \rightarrow E_{\mathbf{k}} + \frac{e}{mc} \mathbf{k} \cdot \mathbf{A}(0) \end{aligned} \quad (52)$$

We may similarly insert the quasiparticle operators (18) into the expression for the expectation value of the paramagnetic current operator(41):

$$\begin{aligned} \langle \mathbf{j}_{para}(\mathbf{q} = 0) \rangle & = \frac{e}{m} \sum_{\mathbf{k}} \langle (\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} - \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1}) \rangle \\ & = \frac{e}{m} \sum_{\mathbf{k}} (f(E_{\mathbf{k}0}) - f(E_{\mathbf{k}1})). \end{aligned} \quad (53)$$

We are interested in the *linear response*  $\mathbf{A} \rightarrow 0$ , so that when we expand wrt  $\mathbf{A}$ , the paramagnetic contribution becomes

$$\langle \mathbf{j}_{para}(\mathbf{q} = 0) \rangle = \frac{2e^2}{m^2 c} \sum_{\mathbf{k}} [\mathbf{k} \cdot \mathbf{A}(0)] \mathbf{k} \left( -\frac{\partial f}{\partial E_{\mathbf{k}}} \right). \quad (54)$$

Combining now with the definition of the response function  $K$  and the diamagnetic current (45), and recalling  $\Sigma_{\mathbf{k}} \rightarrow$

$N_0 \int d\xi_{\mathbf{k}} (d\Omega/4\pi)$ , with  $N_0 = 3n/(2\epsilon_F)$  and  $\int (d\Omega/4\pi) \mathbf{k}\mathbf{k} = \underline{1}/3$ , we get for the static homogeneous response is therefore

$$\underline{K}(0, 0) = \frac{-ne^2}{mc} \{1 - \int d\xi_k \left( \frac{-\partial f}{\partial E_k} \right)\} \underline{1} \quad (55)$$

$$\equiv \frac{-n_s(T)e^2}{mc} \underline{1} \quad (56)$$

where in the last step, I defined the *superfluid density* to be  $n_s(T) \equiv n - n_n(T)$ , with *normal fluid density*

$$\boxed{n_n(T) \equiv n \int d\xi_k \left( \frac{-\partial f}{\partial E_k} \right)}. \quad (57)$$

Note at  $T = 0$ ,  $-\partial f/\partial E_k \rightarrow 0$ , [Not a delta function, as in the normal state case—do you see why?], while at  $T = T_c$  the integral  $n_n \rightarrow 1$ .<sup>11</sup> Correspondingly, the superfluid density as defined varies between  $n$  at  $T = 0$  and 0 at  $T_c$ . This is the BCS microscopic justification for the rather successful phenomenological two-fluid model of superconductivity: the normal fluid consists of the thermally excited Bogoliubov quasiparticle gas, and the superfluid is the condensate of Cooper pairs.<sup>12</sup>

Now let's relate the BCS microscopic result for the static homogeneous response to the penetration depth appearing in the macroscopic electrodynamics calculation above. We find immediately

$$\lambda(T) = \left( \frac{mc^2}{4\pi n_s(T)e^2} \right)^{1/2}. \quad (58)$$

<sup>11</sup>The dimensionless function  $n_n(T/T_c)/n$  is sometimes called the Yoshida function,  $Y(T)$ , and is plotted in Fig.8.

<sup>12</sup>The BCS theory and subsequent extensions also allow one to understand the limitations of the two-fluid picture: for example, when one probes the system at sufficiently high frequencies  $\omega \sim \Delta$ , the normal fluid and superfluid fractions are no longer distinct.

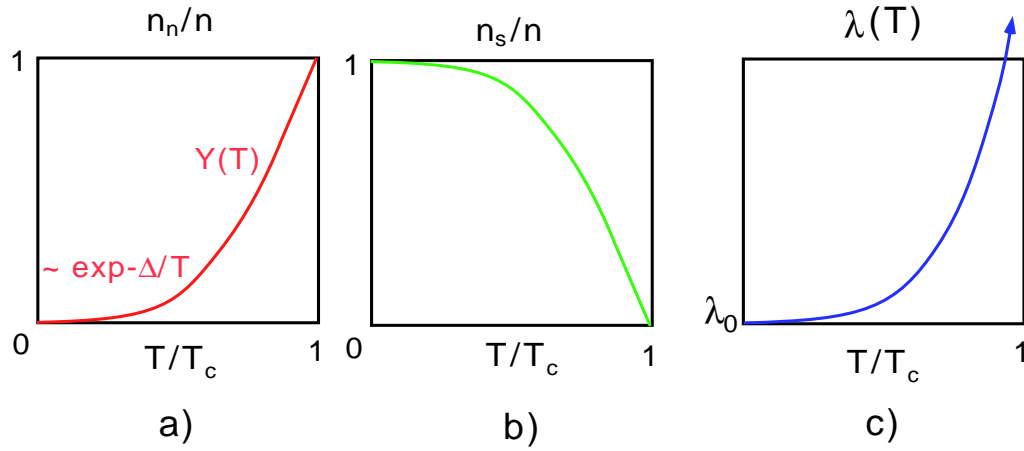


Figure 8: a) Yoshida function; b) superfluid density ; c) penetration depth

At  $T = 0$ , the supercurrent screening excludes the field from all of the sample except a sheath of thickness  $\lambda(0)$ . At small but finite temperatures, an exponentially small number of quasiparticles will be excited out of the condensate, depleting the supercurrent and allowing the field to penetrate further. Both  $n_n(T)$  and  $\lambda(T) - \lambda(0)$  may therefore be expected to vary as  $e^{-\Delta/T}$  for  $T \ll T_c$ , as may be confirmed by explicit expansion of Eq. (57). [See homework.] Close to  $T_c$ , the penetration depth diverges as it must, since in the normal state the field penetrates the sample completely.

### 5.7.3 Dynamical conductivity.

The calculation of the full, frequency dependent conductivity is beyond the scope of this course. If you would like to read an old-fashioned derivation, I refer you to Tinkham's book. The main point to absorb here is that, as in a semiconductor with a gap, at  $T = 0$  there is no process by which a photon can be absorbed in a superconductor until its energy exceeds  $2\Delta$ ,

the binding energy of the pair. This “threshold” for optical absorption is one of the most direct measurements of the gaps of the old superconductors.

## 6 Ginzburg-Landau Theory

### 6.1 GL Free Energy

While the BCS weak-coupling theory we looked at the last two weeks is very powerful, and provides at least a qualitatively correct description of most aspects of classic superconductors,<sup>13</sup> there is a complementary theory which a) is simpler and more physically transparent, although valid only near the transition; and b) provides exact results under certain circumstances. This is the Ginzburg-Landau theory [ V.L. Ginzburg and L.D. Landau, *Zh. Eksp. Teor. Fiz.* 20, 1064 (1950)], which received remarkably little attention in the west until Gor’kov showed it was derivable from the BCS theory. [L.P. Gor’kov, *Zh. Eksp. Teor Fiz.* 36, 1918 (1959)]. The theory simply postulated the existence of a macroscopic quantum wave function  $\psi(r)$  which was equivalent to an order parameter, and proposed that on symmetry grounds alone, the free energy density of a superconductor should be expressible in terms of an expansion in this quantity:

$$\frac{f_s - f_n}{V} = a|\psi|^2 + b|\psi|^4 + \frac{1}{2m^*} |(\nabla + \frac{ie^*}{c}\vec{A})\psi|^2, \quad (59)$$

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<sup>13</sup>In fact one could make a case that the BCS theory is the most quantitatively accurate theory in all of condensed matter physics

where the subscripts n and s refer to the normal and superconducting states, respectively.

Let's see why GL might have been led to make such a “guess”. The superconducting-normal transition was empirically known to be second order in zero field, so it was natural to write down a theory analogous to the Landau theory of a ferromagnet, which is an expansion in powers of the magnetization,  $\mathbf{M}$ . The choice of order parameter for the superconductor corresponding to  $\mathbf{M}$  for the ferromagnet was not obvious, but a complex scalar field  $\psi$  was a natural choice because of the analogy with liquid  $He$ , where  $|\psi|^2$  is known to represent the superfluid density  $n_s$ ;<sup>14</sup> a quantum mechanical density should be a complex wave function squared. The biggest leap of GL was to specify correctly how electromagnetic fields (which had no analog in superfluid  $He$ ) would couple to the system. They exploited in this case the similarity of the formalism to ordinary quantum mechanics, and coupled the fields in the usual way to “charges”  $e^*$  associated with “particles” of mass  $m^*$ . Recall for a real charge in a magnetic field, the kinetic energy is:

$$\langle \Psi | \mathcal{H}_{kin} | \Psi \rangle = -\frac{1}{2m} \int d^3r \Psi^* (\nabla + \frac{ie}{c} \vec{A})^2 \Psi \quad (60)$$

$$= \frac{1}{2m} \int d^3r |(\nabla + \frac{ie}{c} \vec{A}) \Psi|^2, \quad (61)$$

after an integration by parts in the second step. GL just replaced  $e, m$  with  $e^*, m^*$  to obtain the kinetic part of Eq. (59);

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<sup>14</sup> $\psi$  in the  $He$  case has the microscopic interpretation as the Bose condensate amplitude.

they expected that  $e^*$  and  $m^*$  were the elementary electron charge and mass, respectively, but did not assume so.

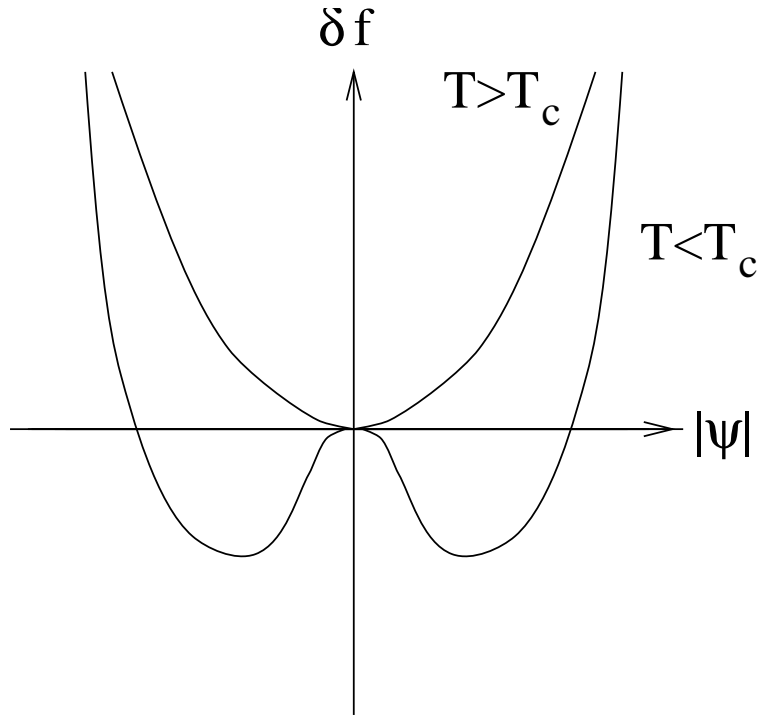


Figure 9: Mexican hat potential for superconductor.

A system described by this free energy will undergo a second-order phase transition in zero field when  $a = 0$ : clearly when  $a$  is positive, the system can minimize  $\delta f$  by having  $\psi = 0$  (no superconductivity), whereas if  $a$  is negative,  $\delta f$  has a minimum with  $\psi \neq 0$ . The free energy (59) is a *functional* of the order parameter  $\psi$ , meaning the actual value of the order parameter realized in equilibrium satisfies  $\delta f / \delta \psi = 0$ .<sup>15</sup> Notice  $f$  is independent of the phase  $\phi$  of the order parameter,  $\psi \equiv |\psi|e^{i\phi}$ , and so the ground state for  $a < 0$  is equivalent to any state  $\psi$  related to it by multiplication by a pure phase. This is the  $U(1)$  gauge invariance of which we spoke earlier.

<sup>15</sup>Thus you should not be perturbed by the fact that  $f$  apparently depends on  $\psi$  even for  $a > 0$ . The value of  $f$  in equilibrium will be  $f_n = f[\psi = 0]$ .

This symmetry is broken when the system chooses one of the ground states (phases) upon condensation (Fig 1.).

For a uniform system in zero field, the total free energy  $F = \int d^3r f$  is minimized when  $f$  is, so one find for the order parameter at the minimum,

$$|\psi|_{eq} = [\frac{-a}{2b}]^{1/2}, \quad a < 0 \quad (62)$$

$$|\psi|_{eq} = 0, \quad a > 0. \quad (63)$$

When  $a$  changes sign, a minimum with a nonzero value becomes possible. For a second order transition as one lowers the temperature, we assume that  $a$  and  $b$  are smooth functions of  $T$  near  $T_c$ . Since we are only interested in the region near  $T_c$ , we take only the leading terms in the Taylor series expansions in this region:  $a(T, H) = a_0(T - T_c)$  and  $b = \text{constant}$ . Eqs. (62) and (63) take the form:

$$|\psi(T)|_{eq} = [\frac{a_0(T_c - T)}{2b}]^{1/2}, \quad T < T_c \quad (64)$$

$$|\psi(T)|_{eq} = 0, \quad T > T_c. \quad (65)$$

Substituting back into Eqs.59, we find:

$$f_s(T) - f_n(T) = -\frac{a_0^2}{4b}(T_c - T)^2, \quad T < T_c \quad (66)$$

$$f_s(T) - f_n(T) = 0, \quad T > T_c. \quad (67)$$

The idea now is to calculate various observables, and determine the GL coefficients for a given system. Once they are determined, the theory acquires predictive power due to its extreme simplicity. It should be noted that GL theory is applied to many systems, but it is in classic superconductors



that it is most accurate, since the critical region, where deviations from mean field theory are large, is of order  $10^{-4}$  or less. Near the transition it may be taken to be exact for all practical purposes. This is not the case for the HTSC, where the size of the critical region has been claimed to be as much as 10-20K in some samples.

**Supercurrents.** Let's now focus our attention on the term in the GL free energy which leads to supercurrents, the kinetic energy part:

$$F_{\text{kin}} = \int d^3r \frac{1}{2m^*} |(\nabla + \frac{ie^*}{c} \vec{A})\psi|^2 \quad (68)$$

$$= \int d^3r \frac{1}{2m^*} [(\nabla|\psi|)^2 + (\nabla\phi - e^*/c\mathbf{A})^2|\psi|^2]. \quad (69)$$

These expressions deserve several remarks. First, note that the free energy is gauge invariant, if we make the transformation  $\vec{A} \rightarrow \vec{A} + \nabla\Lambda$ , where  $\Lambda$  is any scalar function of position, while at the same time changing  $\psi \rightarrow \psi \exp(-ie^*\Lambda/c)$ . Second, note that in the last step above I have split the kinetic part of  $f$  into a term dependent on the gradients of the order parameter magnitude  $|\psi|$  and on the gradients of the phase  $\phi$ . Let us use a little intuition to guess what these terms mean. The energy of the superconducting state below  $T_c$  is lower than that of the normal state by an amount called the *condensation energy*.<sup>16</sup> From Eq. (59) in zero field this is of order  $|\psi|^2$  very close to the transition. To make spatial variations of the *magnitude* of  $\psi$  must cost a significant fraction of the condensation energy in the region of space in which it

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<sup>16</sup>We will see below from the Gorkov derivation of GL from BCS that it is of order  $N(0)\Delta^2$ .

occurs.<sup>17</sup> On the other hand, the zero-field free energy is actually invariant with respect to changes in  $\phi$ , so fluctuations of  $\phi$  alone actually cost no energy.

With this in mind, let's ask what will happen if we apply a weak magnetic field described by  $\mathbf{A}$  to the system. Since it is a small perturbation, we don't expect it to couple to  $|\psi|$  but rather to the phase  $\phi$ . The kinetic energy density should then reduce to the second term in Eq. (69), and furthermore we expect that it should reduce to the intuitive two-fluid expression for the kinetic energy due to supercurrents,  $\frac{1}{2}mn_s v_s^2$ . Recall from the superfluid *He* analogy, we expect  $|\psi|^2 \equiv n_s^*$  to be a kind of density of superconducting electrons, but that we aren't certain of the charge or mass of the “particles”. So let's put

$$f_{\text{kin}} \simeq \frac{1}{2m^*} |(\nabla + \frac{ie^*}{c}\vec{A})\psi|^2 = \int d^3r \frac{1}{2m^*} (\nabla\phi - e^*/c\mathbf{A})^2 |\psi|^2 \equiv \frac{1}{2}m^*n_s^*v_s^2. \quad (70)$$

Comparing with Eq. (xx), we find that the *superfluid velocity* must be

$$\vec{v}_s = \frac{1}{m^*} (\nabla\phi + \frac{e^*}{c}\vec{A}). \quad (71)$$

Thus the gradient of the phase is related to the superfluid velocity, but the vector potential also appears to keep the entire formalism gauge-invariant.

**Meissner effect.** The Meissner effect now follows immediately from the two-fluid identifications we have made. The

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<sup>17</sup>We can make an analogy with a ferromagnet, where if we have a *domain wall* the magnetization must go to zero at the domain boundary, costing lots of surface energy.

supercurrent density will certainly be just

$$\vec{j}_s = -e^* n_s^* \vec{v}_s = -\frac{e^* n_s^*}{m^*} (\nabla \phi + \frac{e^*}{c} \vec{A}). \quad (72)$$

Taking the curl of this equation, the phase drops out, and we find the magnetic field:

$$\nabla \times \vec{j}_s = -\frac{e^{*2} n_s^*}{m^* c} \vec{B}. \quad (73)$$

Now recall the Maxwell equation

$$\vec{j}_s = \frac{c}{4\pi} \nabla \times \vec{B}, \quad (74)$$

which, when combined with (14), gives

$$\frac{c}{4\pi} \nabla \times \nabla \times \vec{B} = -\frac{c}{4\pi} \nabla^2 \vec{B} = -\frac{e^{*2} n_s^*}{m^* c} \vec{B}, \quad (75)$$

or

$$\lambda^2 \nabla^2 \vec{B} = \vec{B}, \quad (76)$$

where

$$\lambda = \frac{m^* c^2}{4\pi e^{*2} n_s^*}^{1/2}. \quad (77)$$

Notice now that if we use what we know about Cooper pairs, this expression reduces to the BCS/London penetration depth. We assume  $e^*$  is the charge of the pair, namely  $e^* = 2e$ , and similarly  $m^* = 2m$ , and  $|\psi|^2 = n_s^* = n_s/2$  since  $n_s^*$  is the density of pairs.

**Flux quantization.** If we look at the flux quantization described in Part 1 of these notes, it is clear from our subsequent discussion of the Meissner effect, that the currents

which lead to flux quantization will only flow in a small part of the cross section, a layer of thickness  $\lambda$ . This layer encloses the flux passing through the toroid. Draw a contour  $C$  in the interior of the toroid, as shown in Figure 10. Then  $v_s = 0$  everywhere on  $C$ . It follows that

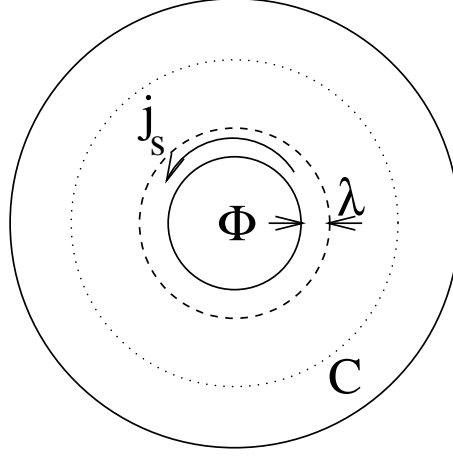


Figure 10: Quantization of flux in a toroid.

$$0 = \oint_C d\vec{\ell} \cdot \vec{v}_s = \frac{1}{m^*} \oint_C d\vec{\ell} \cdot (\nabla \phi + \frac{e^*}{c} \vec{A}). \quad (78)$$

The last integral may be evaluated using

$$\oint_C d\vec{\ell} \cdot \nabla \phi = 2\pi \times integer, \quad (79)$$

and

$$\frac{e^*}{c} \oint_C d\vec{\ell} \cdot \vec{A} = \frac{e^*}{c} \int_S d\vec{S} \cdot \nabla \times \vec{A} \quad (80)$$

$$= \frac{e^*}{c} \int_S d\vec{S} \cdot \vec{B} \quad (81)$$

$$= \frac{e^*}{c} \Phi. \quad (82)$$

Here  $S$  is a surface spanning the hole and  $\Phi$  the flux through

the hole. Combining these results,

$$\Phi = 2\pi \frac{\hbar c}{2e} n = n \frac{hc}{2e} = n\Phi_0, \quad (83)$$

where  $n$  is an integer,  $\Phi_0$  is the flux quantum, and I've reinserted the correct factor of  $\hbar$  in the first step to make the units right. Flux quantization indeed follows from the fact that the current is the result of a phase gradient.<sup>18</sup>

**Derivation from Microscopic Theory.** One of the reasons the GL theory did not enjoy much success at first was the fact that it is purely phenomenological, in the sense that the parameters  $a_0, b, m^*$  are not given within any microscopic framework. The BCS theory is such a framework, and gives values for these coefficients which set the scale for all quantities calculable from the GL free energy. The GL theory is more general, however, since, e.g. for strong coupling superconductors the weak coupling values of the coefficients are simply replaced by different ones of the same order of magnitude, without changing the *form* of the GL free energy. In consequence, the dependence of observables on temperature, field, etc, will obey the same universal forms.

The GL theory was derived from BCS by Gor'kov. The calculation is beyond the scope of this course, but can be found in many texts.

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<sup>18</sup>It is important to note, however, that a phase gradient doesn't guarantee that a current is flowing. For example, in the interior of the system depicted in Fig. 2, both  $\nabla\phi$  and  $\vec{A}$  are nonzero in the most convenient gauge, and cancel each other!

## 6.2 Type I and Type II superconductivity

Now let's look at the problem of the instability of the normal state to superconductivity in finite magnetic field  $\mathbf{H}$ . At what magnetic field do we expect superconductivity to be destroyed, for a given  $T < T_c$ .<sup>19</sup> Well, overall energy is conserved, so the total condensation energy of the system in zero field,  $f_s - f_n(T)$  of the system must be equal to the magnetic field energy  $\int d^3r H^2/8\pi$  the system *would have* contained at the critical field  $H_c$  in the absence of the Meissner effect. For a completely homogeneous system I then have

$$f_s(T) - f_n(T) = -H_c^2/8\pi, \quad (84)$$

and from Eq. (8) this means that, near  $T_c$ ,

$$H_c = \sqrt{\frac{2\pi a_0^2}{b}}(T_c - T). \quad (85)$$

Whether this *thermodynamic critical field*  $H_c$  actually represents the applied field at which flux penetrates the sample depends on geometry. We assumed in the simplified treatment above that the field at the sample surface was the same as the applied field. Clearly for any realistic sample placed in a field, the lines of field will have to follow the contour of the sample if it excludes the field from its interior. This means the value of  $\mathbf{H}$  at different points on the surface will be different: the homogeneity assumption we made will not quite hold. If we imagine ramping up the applied field from

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<sup>19</sup>Clearly it *will* destroy superconductivity since it breaks the degeneracy of between the two components of a Cooper pair.

zero, there will inevitably come a point  $\mathbf{H}_{appl} = \mathbf{H}_{appl,c}$  where the field at certain points on the sample surface exceeds the critical field, but at other points does not. For applied fields  $H_{appl,c} < H_{appl} < H_c$ , part of the sample will then be normal, with local field penetration, and other parts will still exclude field and be superconducting. This is the *intermediate state* of a type I superconductor. The structure of this state for a real sample is typically a complicated "striped" pattern of superconducting and normal phases. Even for small fields, edges and corners of samples typically go normal because the field lines bunch up there; these are called "demagnetizing effects", and must be accounted for in a quantitatively accurate measurement of, say, the penetration depth. It is important to note that these patterns are completely geometry dependent, and have no intrinsic length scale associated with them.

In the 50's, there were several materials known, however, in which the flux in sufficiently large fields penetrated the sample in a manner which did *not* appear to be geometry dependent. For example, samples of these so-called "type II" superconductors with nearly zero demagnetizing factors (long thin plates placed parallel to the field) also showed flux penetration in the superconducting state. The type-II materials exhibit a second-order transition at finite field and the flux  $\mathbf{B}$  through the sample varies continuously in the superconducting state. Therefore the mixed state must have currents flowing, and yet the Meissner effect is not realized, so that the London equation somehow does not hold.

The answer was provided by Abrikosov in 1957 [A.A.A., Sov. Phys. JETP 5, 1174 (1957).] in a paper which Landau apparently held up for several years because he did not believe it. Let us neglect the effects of geometry again, and go back to our theorist's sample with zero demagnetizing factor. Can we relax any of the assumptions that led to the London equation (72)? Only one is potentially problematic, that  $n_s^*(r) = |\psi(r)|^2 = \text{constant}$  independent of position. Let's examine—as Abrikosov did—the energy cost of making spatial variations of the order parameter. The free energy in zero field is

$$F = \int d^3r [a|\psi|^2 + \frac{1}{2m^*}|\nabla\psi|^2 + b|\psi|^4], \quad (86)$$

or

$$\frac{1}{-a}F = \int d^3r [-|\psi|^2 + \xi^2|\nabla\psi|^2 + \frac{b}{-a}|\psi|^4], \quad (87)$$

where I've put

$$\xi = \left[ \frac{1}{-2m^*a} \right]^{1/2} = \left[ \frac{1}{-2m^*a_0(T_c - T)} \right]^{1/2}. \quad (88)$$

Clearly the length  $\xi$  represents some kind of *stiffness* of the quantity  $|\psi|^2$ , the superfluid density. [Check that it does indeed have dimensions of length!] If  $\xi$ , the so-called *coherence length*, is small, the energy cost of  $n_s$  varying from place to place will be small. If the order parameter is somehow changed from its homogeneous equilibrium value at one point in space by an external force,  $\xi$  specifies the length scale over which it "heals". We can then investigate the possibility that, as the kinetic energy of superfluid flow increases with increasing



field, if  $\xi$  is small enough it might eventually become favorable to "bend"  $|\psi|^2$  instead. In typical type I materials,  $\xi(T = 0)$  is of order several hundreds or even thousands of Angstrom, but in heavy fermion superconductors, for example, coherence lengths are of order 50-100Å. The smallest coherence lengths are attained in the HTSC, where  $\xi_{ab}$  is of order 12-15Å, whereas  $\xi_c$  is only 2-3Å.

The general problem of minimizing  $F$  when  $\psi$  depends on position is extremely difficult. However, we are mainly interested in the phase boundary where  $\psi$  is small, so life is a bit simpler. Let's recall our quantum mechanics analogy once more so as to write  $F$  in the form:

$$F = \int d^3r [a|\psi|^2 + b|\psi|^4] + \langle \psi | \hat{H}_{kin} | \psi \rangle, \quad (89)$$

where  $\hat{H}_{kin}$  is the operator

$$-\frac{1}{2m^*}(\nabla + \frac{ie^*}{c}\vec{A})^2. \quad (90)$$

Now note 1) sufficiently close to the transition, we may always neglect the 4th-order term, which is much smaller; 2) to minimize  $F$ , it suffices to minimize  $\langle \hat{H}_{kin} \rangle$ , since the  $|\psi|^2$  term will simply fix the overall normalization. The variational principle of quantum mechanics states that the minimum value of  $\langle H \rangle$  over all possible  $\psi$  is achieved when  $\psi$  is the ground state (for a given normalization of  $\psi$ ). So we need only solve the eigenvalue problem

$$\hat{H}_{kin}\psi_j = E_j\psi_j \quad (91)$$

for the lowest eigenvalue,  $E_j$ , and corresponding eigenfunction  $\psi_j$ . For the given form of  $\hat{H}_{kin}$ , this reduces to the classic quantum mechanics problem of a charged particle moving in an applied magnetic field. The applied field  $H$  is essentially the same as the microscopic field  $B$  since  $\psi$  is so small (at the phase boundary only!). I'll remind you of the solution, due to Landau, in order to fix notation. We choose a convenient gauge,

$$\mathbf{A} = -Hy\hat{x}, \quad (92)$$

in which Eq. 44 becomes

$$\frac{1}{2m^*} \left[ \left( -i\frac{\partial}{\partial x} + \frac{y}{\ell_M^2} \right)^2 - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \right] \psi_j = E_j \psi_j, \quad (93)$$

where  $\ell_M = (c/e^*H)^{1/2}$  is the *magnetic length*. Since the coordinates  $x$  and  $z$  don't appear explicitly, we make the ansatz of a plane wave along those directions:

$$\psi = \eta(y) e^{ik_x x + ik_z z}, \quad (94)$$

yielding

$$\frac{1}{2m^*} \left[ \left( k_x + \frac{y}{\ell_M^2} \right)^2 - \frac{\partial^2}{\partial y^2} + k_z^2 \right] \eta(y) = E \eta(y). \quad (95)$$

But this you will recognize as just the equation for a one-dimensional harmonic oscillator centered at the point  $y = -k_x \ell_M^2$  with an additional additive constant  $k_z^2/2m^*$  in the energy. Recall the standard harmonic oscillator equation

$$\left( -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} k x^2 \right) \Psi = E \Psi, \quad (96)$$

with ground state energy

$$E_0 = \frac{\omega_0}{2} = \frac{1}{2}(k/m)^{1/2}, \quad (97)$$

where  $k$  is the spring constant, and ground state wavefunction corresponding to the lowest order Hermite polynomial,

$$\Psi_0 \approx \exp[-(mk/4)^{1/2}x^2]. \quad (98)$$

Let's just take over these results, identifying

$$\hat{H}_{kin}\psi_{k_x,k_z} = \frac{e^*H}{2m^*c}\psi_{k_x,k_z}. \quad (99)$$

The ground state eigenfunction may then be chosen as

$$\psi_{k_x,k_z} = \psi_0 \left(\frac{\pi\ell_M^2}{L_y^2}\right)^{-1/4} e^{ik_x x + ik_z z} \exp[-(y + k_x \ell_M^2)^2 / 2\ell_M^2], \quad (100)$$

where  $L_y$  is the size of the sample in the  $y$  direction ( $L_x L_y L_z = V = 1$ ). The wave functions are normalized such that

$$\int d^3r |\psi_{k_x,k_z}|^2 = \psi_0^2 \quad (101)$$

(since I set the volume of the system to 1). The prefactors are chosen such that  $\psi_0^2$  represents the average superfluid density. One important aspect of the particle in a field problem seen from the above solution is the large degeneracy of the ground state: the energy is independent of the variable  $k_x$ , for example, corresponding to many possible orbit centers.

We have now found the wavefunction which minimizes  $\langle \hat{H}_{kin} \rangle$ . Substituting back into (89), we find using (99)

$$F = [a_0(T - T_c) + \frac{e^*H}{2m^*c}] \int d^3r |\psi|^2 + b \int d^3r |\psi|^4. \quad (102)$$

When the coefficient of the quadratic term changes sign, we have a transition. The field at which this occurs is called the *upper critical field*  $H_{c2}$ ,

$$H_{c2}(T) = \frac{2m^*ca_0}{e^*}(T_c - T). \quad (103)$$

What is the criterion which distinguishes type-I and type II materials? Start in the normal state for  $T < T_c$  as shown in Figure 3, and reduce the field. Eventually one crosses either  $H_c$  or  $H_{c2}$  first. Whichever is crossed first determines the nature of the instability in finite field, i.e. whether the sample expels all the field, or allows flux (vortex) penetration (see section C).

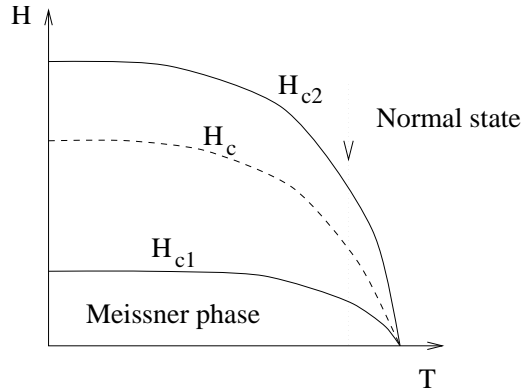


Figure 11: Phase boundaries for classic type II superconductor.

In the figure, I have displayed the situation where  $H_{c2}$  is higher, meaning it is encountered first. The criterion for the dividing line between type 1 and type II is simply

$$\left| \frac{dH_c}{dT} \right| = \left| \frac{dH_{c2}}{dT} \right| \quad (104)$$

or, using the results (38) and (56),

$$\frac{(m^*)^2 c^2 b}{\pi (e^*)^2} = \frac{1}{2}. \quad (105)$$

This criterion is a bit difficult to extract information from in its current form. Let's define the *GL parameter*  $\kappa$  to be the ratio of the two fundamental lengths we have identified so far, the penetration depth and the coherence length:

$$\kappa = \frac{\lambda}{\xi}. \quad (106)$$

Recalling that

$$\lambda^2 = -\frac{m^* c^2}{4\pi e^{*2} n_s^*} = -\frac{m^* c^2 b}{2\pi e^{*2} a} \quad (107)$$

and

$$\xi^2 = -\frac{1}{2m^* a}. \quad (108)$$

The criterion (58) now becomes

$$\kappa^2 = \frac{m^* c^2 b / 2\pi e^{*2} a}{1/2m^* a} = \frac{(m^*)^2 c^2 b}{\pi e^{*2}} = \frac{1}{2}. \quad (109)$$

Therefore a material is type I (II) if  $\kappa$  is less than (greater than)  $\frac{1}{\sqrt{2}}$ . In type-I superconductors, the coherence length is large compared to the penetration depth, and the system is stiff with respect to changes in the superfluid density. This gives rise to the Meissner effect, where  $n_s$  is nearly constant over the screened part of the sample. Type-II systems can't screen out the field close to  $H_{c2}$  since their stiffness is too

small. The screening is incomplete, and the system must decide what pattern of spatial variation and flux penetration is most favorable from an energetic point of view. The result is the *vortex lattice* first described by Abrikosov.

### 6.3 Vortex Lattice

I commented above on the huge degeneracy of the wave functions (53). In particular, for fixed  $k_z = 0$ , there are as many ground states as allowed values of the parameter  $k_x$ . At  $H_{c2}$  it didn't matter, since we could use the eigenvalue alone to determine the phase boundary. Below  $H_{c2}$  the fourth order term becomes important, and the minimization of  $f$  is no longer an eigenvalue problem. Let's make the plausible assumption that if some spatially varying order parameter structure is going to form below  $H_{c2}$ , it will be periodic with period  $2\pi/q$ , i.e. the system *selects* some wave vector  $\mathbf{q}$  for energetic reasons. The  $x$ -dependence of the wave functions

$$\psi_{k_x, k_z=0} = \psi_0 \left( \frac{\pi \ell_M^2}{L_y^2} \right)^{-1/4} e^{ik_x x} \exp[-(y + k_x \ell_M^2)^2 / 2\ell_M^2]. \quad (110)$$

is given through plane wave phases,  $e^{ik_x x}$ . If we choose  $k_x = qn_x$ , with  $n_x = \text{integer}$ , all such functions will be invariant under  $x \rightarrow x + 2\pi/q$ . Not all  $n_x$ 's are allowed, however: the center of the "orbit",  $k_x \ell_M^2$  should be inside the sample:

$$-L_y/2 < k_x \ell_M^2 = q \ell_M^2 n_x < L_y/2, \quad (111)$$

Thus  $n_x$  is restricted such that

$$-\frac{L_y}{2q\ell^2} = -n_{max}/2 < n_x < n_{max}/2 = \frac{L_y}{2q\ell^2} \quad (112)$$

and the total number of degenerate functions is  $L_y/(q\ell_M^2)$ .

Clearly we need to build up a periodic spatially varying structure out of wave functions of this type, with "centers" distributed somehow. What is the criterion which determines this structure? All the wave functions (110) minimize  $\langle \hat{H}_{kin} \rangle$ , and are normalized to  $\int d^3r |\psi|^2 = |\psi_0|^2$ . They are all therefore degenerate at the level of the quadratic GL free energy,  $F = \int d^3r |\psi|^2 + \langle \hat{H}_{kin} \rangle$ . The fourth order term must stabilize some linear combination of them. We therefore write

$$\psi(r) = \sum_{n_x} C_{n_x} \psi_{n_x}(r), \quad (113)$$

with the normalization  $\sum_{n_x} |C_{n_x}|^2 = 1$ , which enforces  $\int d^3r |\psi(r)|^2 = \psi_0^2$ . Note this must minimize  $\langle \hat{H}_{kin} \rangle$ . Let's therefore choose the  $C_{n_x}$  and  $q$  to minimize the remaining terms in  $F$ ,  $\int d^3r [a|\psi|^2 + b|\psi|^4]$ . Substituting and using the normalization condition and orthogonality of the different  $\psi_{k_z, k_x}$ , we find

$$f = \tilde{a}\psi_0^2 + \tilde{b}\psi_0^4. \quad (114)$$

with

$$\tilde{a}(H, T) = a_0(T - T_c) + \frac{e^* H}{2m^* c} = \frac{e^*}{2m^* c} (H - H_{c2}(T)), \quad (115)$$

$$\tilde{b}(H) = sb, \quad (116)$$

and

$$s = \left(\frac{\pi\ell_M^2}{L_y^2}\right)^{-1} \sum_{n_{x1}, n_{x2}, n_{x3}, n_{x4}}^{n_{max}} C_{n_{x1}}^* C_{n_{x2}}^* C_{n_{x3}} C_{n_{x4}} \quad (117)$$

$$\int dz \int dx e^{iq(-n_{x1}-n_{x2}+n_{x3}+n_{x4})x} \times \quad (118)$$

$$\int dy e^{\{-\frac{1}{2\ell_M^2}[(y+qn_{x1}\ell_M^2)^2+(y+qn_{x2}\ell_M^2)^2+(y+qn_{x3}\ell_M^2)^2+(y+qn_{x4}\ell_M^2)^2]\}} \quad (119)$$

The *form* of  $f[\psi_0]$  is now the same as in zero field, so we immediately find that in equilibrium,

$$\psi_0|_{eq} = \left(\frac{-\tilde{a}}{2\tilde{b}}\right)^{1/2}. \quad (120)$$

and

$$f = \frac{-\tilde{a}^2}{4\tilde{b}}. \quad (121)$$

This expression depends on the variational parameters  $C_{n_x}, q$  only through the quantity  $s$  appearing in  $\tilde{b}$ . Thus if we minimize  $s$ , we will minimize  $f$  (remember  $b > 0$ , so  $f < 0$ ). The minimization of the complicated expression (xx) with constraint  $\sum_{n_x} |C_{n_x}|^2 = 1$  is difficult enough that A. Abrikosov made a mistake the first time he did it, and I won't inflict the full solution on you. To get an idea what it might look like, however, let's look at a very symmetric linear combination, one where all the  $C_{n_x}$ 's are equal:

$$C_n = n_{max}^{-1/2}. \quad (122)$$

Then

$$\psi(r) \sim \sum_n e^{inqx} \exp[-(y + nq\ell^2)^2/2\ell_M^2], \quad (123)$$

which is periodic in  $x$  with period  $2\pi/q$ ,

$$\psi(x + 2\pi/q, y) = \psi(x, y), \quad (124)$$

and periodic in  $q$  with period  $q\ell_M^2$ , up to a phase factor

$$\psi(x, y + q\ell_M^2) = e^{-iqx}\psi(x, y). \quad (125)$$



Note if  $q = \sqrt{2\pi}/\ell_M$ ,  $|\psi|^2$  forms a square lattice! The area of a unit cell is  $(2\pi/q) \times (q\ell_M^2) = 2\pi\ell_M^2$ , and the flux through each one is therefore

$$\Phi_{cell} = 2\pi\ell_M^2 H = 2\pi \frac{c}{e^* H} H = \frac{hc}{2e} = \Phi_0 \quad (126)$$

where I inserted a factor of  $\hbar$  in the last step. We haven't performed the minimization explicitly, but this is a characteristic of the solution, that each cell contains just one flux quantum. The picture is crudely depicted in Fig. 12a). Note by symmetry that the currents must cancel on the boundaries

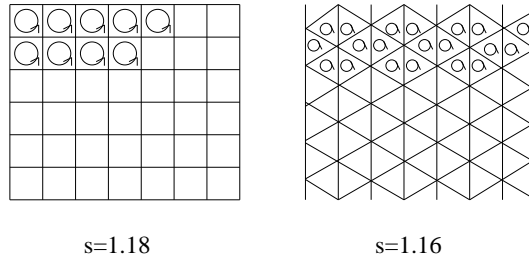


Figure 12: a) Square vortex lattice; b) triangular vortex lattice.

of the cells. Since  $\vec{j}_s = -en_s \vec{v}_s$ , integrating  $\nabla\phi + \frac{2e}{\hbar c} \vec{A} = 0$  around each square must give, as in our previous discussion of flux quantization in a toroid,

$$\Phi_{cell} = n\Phi_0, n = integer. \quad (127)$$

Somehow the vortex lattice consists of many such rings. The problem with this idea is that the only way  $\oint \nabla\phi \cdot d\vec{\ell} = \delta\phi$  around the boundary can be nonzero and the usual argument about single-valuedness of the wave function carried through is if there is a “hole” in the wave function. If there is no hole, or region from which the wave function is excluded, the path can be shrunk to a point, but the value of the integral must

remain the same since the integrand is the gradient of a scalar field. This is unphysical because it would imply a finite phase change along an infinitesimal path (and a divergence of the kinetic energy!) The only way out of the paradox is to have the system introduce its own “hole” in itself, i.e. have the amplitude of the order parameter density  $|\psi|^2$  go to zero at the center of each cell. Intuitively, the magnetic field will have an accompanying maximum here, since the screening tendency will be minimized. This reduction in order parameter amplitude, magnetic flux bundle, and winding of the phase once by  $2\pi$  constitute a magnetic “vortex”, which I’ll discuss in more detail next time.

Assuming  $C_n = \text{constant}$ , which leads to the square lattice does give a relatively good (small) value for the dimensionless quantity  $s$ , which turns out to be 1.18. This was Abrikosov’s claim for the absolute minimum of  $f[|\psi|^2]$ . But his paper contained a (now famous) numerical error, and it turns out that the actual minimum  $s = 1.16$  is attained for another set of the  $C_n$ ’s, to wit

$$C_n = n_{max}^{-1/2}, \quad n = \text{even} \quad (128)$$

$$C_n = in_{max}^{-1/2}, \quad n = \text{odd}. \quad (129)$$

This turns out to be a *triangular* lattice (Fig. 12b), for which the optimal value of  $q$  is found to be

$$q = \frac{3^{1/4}\pi^{1/2}}{\ell}, \quad (130)$$

Again the area of the unit cell is  $2\pi\ell^2$ , and there is one flux

quantum per unit cell.

#### 6.4 Properties of Single Vortex. Lower critical field $H_{c1}$

Given that the flux per unit cell is quantized, it is very easy to see that the lattice spacing  $d$  is actually of order the coherence length near  $H_{c2}$ . Using (103) and (88) we have

$$H_{c2} = \frac{c}{e^*} \frac{1}{\xi^2} = \frac{\Phi_0}{2\pi\xi^2}. \quad (131)$$

On the other hand, as  $H$  is reduced,  $d$  must increase. To see this, note that the area of the triangular lattice unit cell is  $A = \sqrt{3}d^2/2$ , and that there is one quantum of flux per cell,  $A = \Phi_0/H$ . Then the lattice constant may be expressed as

$$d = \frac{4\pi}{\sqrt{3}}\xi\left(\frac{H_{c2}}{H}\right)^{1/2}. \quad (132)$$

Since  $\lambda \gg \xi$  is the length scale on which supercurrents and magnetic fields vary, we expect the size of a magnetic vortex to be about  $\lambda$ . This means at  $H_{c2}$  vortices are strongly overlapping, but as the field is lowered, the vortices separate, according to (126), and may eventually be shown to influence each other only weakly. To find the structure of an isolated vortex is a straightforward but tedious exercise in minimizing the GL free energy, and in fact can only be done numerically in full detail. But let's exploit the fact that we are interested primarily in strongly type-II systems, and therefore go back to the London equation we solved to find the penetration

depth in the half-space geometry for weak fields, allow  $n_s$  to vary spatially, and look for vortex-like solutions. For example, equation (75) may be written

$$-\lambda^2 \nabla \times \nabla \times \vec{B} = \vec{B}. \quad (133)$$

Let's integrate this equation over a surface perpendicular to the field  $\vec{B} = \vec{B}(x, y) \hat{z}$  spanning one cell of the vortex lattice:

$$-\lambda^2 \int \nabla \times (\nabla \times \vec{B}) \cdot d\vec{S} = \int \vec{B} \cdot d\vec{S}, \quad (134)$$

$$-\lambda^2 \frac{4\pi}{c} \oint \vec{j}_s \cdot d\vec{\ell} = \Phi_0. \quad (135)$$

But we have already argued that  $\vec{j}_s \cdot d\vec{\ell}$  should be zero on the boundary of a cell, so the left side is zero and there is a contradiction. What is wrong? The equation came from assuming a two-fluid hydrodynamics for the superconductor, with a nonzero  $n_s$  everywhere. We derived it, in fact, from BCS theory, but *only for the case where  $n_s$  was constant*. Clearly there must be another term in the equation when a vortex-type solution is present, one which can only contribute over the region where the superfluid density is strongly varying in space, i.e. the coherence length-sized region in the middle of the vortex where the order parameter goes to zero (vortex “core”). Let's simply add a term which enables us to get the right amount of flux to Eq. (133). In general we should probably assume something like

$$\lambda^2 \nabla \times \nabla \times \vec{B} + \vec{B} = \Phi_0 g(\vec{r}) \hat{z} \quad (136)$$

where  $g(r)$  is some function which is only nonzero in the core. The flux will then come out right if we demand  $\int d^3r g(\vec{r}) =$

1. But let's simplify things even further, by using the fact that  $\xi \ll \lambda$ : let's treat the core as having negligible size, which means it is just a *line singularity*. We therefore put  $g(\vec{r}) = \delta(\vec{r})$ . Then the modified London equation with line singularity acting as an inhomogeneous “source term” reads

$$-\lambda^2 \nabla^2 \vec{B} + \vec{B} = \Phi_0 \delta^2(\vec{r}) \hat{z} \quad (137)$$

$$-\lambda^2 \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial B_z}{\partial \rho} \right) + B_z = \Phi_0 \delta^2(\vec{r}), \quad (138)$$

where  $\rho$  is the radial cylindrical coordinate. Equation (91) has the form of a modified Bessel's equation with solution:

$$B_z = \frac{\Phi_0}{2\pi\lambda^2} K_0\left(\frac{\rho}{\lambda}\right). \quad (139)$$

The other components of  $\vec{B}$  vanish. If you go to Abramowitz & Stegun you can look up the asymptotic limits:

$$B_z = \frac{\Phi_0}{2\pi\lambda^2} \left[ \log\left(\frac{\lambda}{\rho}\right) + 0.116 \right], \quad \xi < \rho \ll \lambda \quad (140)$$

$$B_z = \frac{\Phi_0}{2\pi\lambda^2} \sqrt{\frac{\pi\lambda}{2\rho}} e^{-\rho/\lambda}, \quad \rho \gg \lambda. \quad (141)$$

Note the form (93) is actually the correct asymptotic solution to (91) all the way down to  $\rho = 0$ , but the fact that the solution diverges logarithmically merely reflects the fact that we didn't minimize the free energy properly, and allow the order parameter to relax as it liked within the core. So the domain of validity of the solution is only down to roughly the core size,  $\rho \simeq \xi$ , as stated. In Figure 5 I show schematically the structure of the magnetic and order parameter profiles in

an isolated vortex. The solution may now be inserted into the

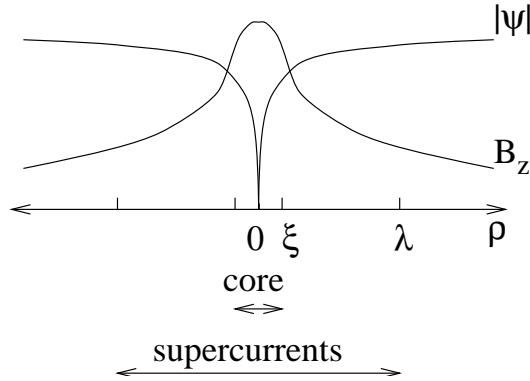


Figure 13: Isolated vortex

free energy and the spatial integrals performed, with some interesting results:

$$F = L_z \frac{\Phi_0^2}{16\pi^2 \lambda^2} \log(\kappa). \quad (142)$$

It is easy to get an intuitive feel for what this means, since if we assume the field is uniform and just ask what is the magnetic energy, we get roughly

$$F_v = \frac{1}{8\pi} \times \text{vortex volume} \times B^2 \quad (143)$$

$$\simeq \frac{1}{8\pi} \times (\pi \lambda^2 L_z) \times (\Phi_0 / \pi \lambda^2)^2 \quad (144)$$

$$= L_z \frac{\Phi_0^2}{8\pi^2 \lambda^2}, \quad (145)$$

the same result up to a slowly varying factor. Now the *lower critical field*  $H_{c1}$  is determined by requiring the Gibbs free energies of the Meissner phase with no vortex be equal to the Gibbs free energy of the phase with a vortex.<sup>20</sup>  $G$  differs from

<sup>20</sup>We haven't talked about the Gibbs vs. Helmholtz free energy, but recall the Gibbs is the appropriate potential to use when the external field  $H$  is held fixed, which is the situation we always have, with a generator supplying work to maintain  $H$ .

$F$  through a term  $-\int BH/4\pi$ . In the Meissner state  $G = F$ , so we may put

$$F = F + E_{line}L_z - \frac{1}{4\pi}H_{c1} \int B d^3r \quad (146)$$

$$= F + E_{line}L_z - \frac{1}{4\pi}\Phi_0 L_z, \quad (147)$$

where  $E_{line}$  is the free energy per unit length of the vortex itself. Therefore

$$H_{c1} = \frac{4\pi E_{line}}{\Phi_0} \quad (148)$$

is the upper critical field. But the line energy is given precisely by Eq. (95),  $E_{line} = \frac{\Phi_0^2}{16\pi^2\lambda^2} \log(\kappa)$ , so

$$H_{c1}(T) = \frac{\Phi_0}{4\pi\lambda^2} \log(\kappa). \quad (149)$$

## 6.5 Josephson Effect

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# 6 Quantum Transport

## 6.1 Disordered metals

In this course we have thus far largely discounted the effects of disorder, which are of course vitally important for the understanding of real experiments. Understanding why under some circumstances we are allowed to ignore disorder is as important as understanding why we are sometimes allowed to ignore electron-electron interactions. Indeed, work on the two subjects (disorder and interactions) has been pursued independently for several decades, with only a few noteworthy attempts to solve the problems of celebrated difficulty which involve both. A great breakthrough on the problem of disorder in 2 and 3D came in 1979, with the application of renormalization group ideas to the localization problem (“Gang of 4”, Licciardello et al 1979).<sup>1</sup> Ideas from this work are key to debates going on today in the 2D metal-insulator transition area and others. I am going to try to lead you through the physical ideas necessary to understand this breakthrough and its implications.

First we review briefly the notion of a metal-insulator transition. This we take to be a phase transition which separates two physical regions which differ in their electrical DC conductivities at zero temperature  $\sigma(\omega = 0, T = 0) \equiv \sigma(0)$ . A metal has finite conductivity  $\sigma(0)$ , while an insulator is characterized by  $\sigma(0) = 0$ . You already know an example of this

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<sup>1</sup>Disorder in 1D has its own special ideas and terminology, which I will only briefly touch on here.

type of transition which does not involve disorder at all: the Mott transition which takes place, e.g. in the Hubbard model at half-filling due to interactions. In that case the parameter one tunes is the on-site Coulomb interaction  $U$  to go from the metallic (small  $U$ ) to insulating (large  $U$ ) state. I'm going to stick to discussing metal insulator transition in noninteracting disordered systems, sometimes referred to as the Anderson transition. By “disorder”, one means the deviation from strict lattice periodicity due to impurities or defects.<sup>2</sup>

### 6.1.1 Boltzmann equation for impurities

The semiclassical theory of transport you learned last semester is based on a key assumption, which is often swept under the rug, namely that the mean free path due to whatever scattering processes one is considering, is longer than the Fermi wavelength. Here I'll eventually give a review of Boltzmann results on impurity-limited transport. See Ashcroft & Mermin Ch. 12 for now.

Reminder: Drude Conductivity. At  $T = 0$ , there is no inelastic scattering due to phonons or  $e^- - e^-$  collisions; in fact in an unbounded, periodic lattice no scattering occurs at all, and the system has infinite conductivity; this is a consequence of quantum mechanics. We could equally well say that the collision time  $\tau$  for scattering, or the mean free path  $\ell = v_F \tau$  are infinite. The wavefunction of a particle in such a case is

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<sup>2</sup>These defects can be so numerous that it no longer makes sense to think of small deviations from periodicity, in which case the word “amorphous” is sometimes used.



**Claim:** when we make the system more disordered, the wave function may become *localized*, i.e. the particle gets trapped. This is signalled by

$$|\psi(\mathbf{r})|^2 \propto e^{-r/\xi}, \quad (3)$$

where  $\xi$  is the *localization length*. How disordered does a system have to get for this to occur? To quantify the claim, we consider a specific 1D model, generalize the Kronig-Penney model of an electron moving in a periodic  $\delta$ -function lattice to a set of  $\delta$ -function potentials of strength  $V_i$  at random positions  $x_i$ , with separations  $a_i$ . The potential is then given

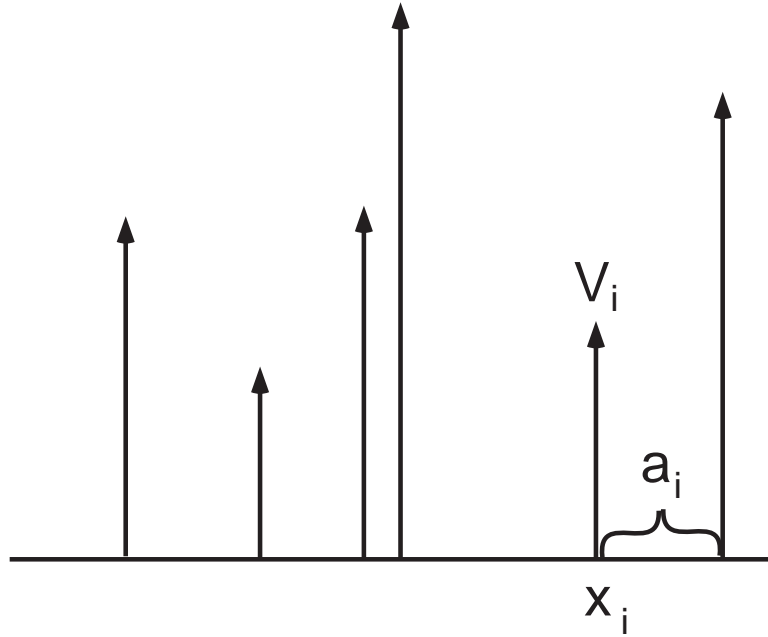


Figure 2: Generalized Kronig-Penney model of 1D disordered solid.

by

$$V(x) = \frac{1}{2m} \sum_i V_i \delta(x - x_i), \quad (4)$$

so the Schrödinger eqn. becomes

$$\left[ -\nabla^2 + \sum_i V_i \delta(x - x_i) - k^2 \right] \psi(x) = 0 \quad (5)$$

with  $k^2 = \sqrt{2mE}$ . Imagine one of these peaks is located at the origin. The wave functions  $\psi_{\pm}(x)$  for  $x \gtrless 0$  are then

$$\psi_{\pm} = A_{\pm}e^{ikx} + B_{\pm}e^{-ikx}. \quad (6)$$

The boundary conditions at  $x = 0$  for the wave functions and spatial derivatives are then

$$\begin{aligned} \psi_+(0) &= \psi_-(0) \\ \psi'_+(0) &= \psi'_-(0) + V_0\psi(0), \end{aligned} \quad (7)$$

Now we look for a solution which is *periodic*, such that  $|\psi_+(a)|^2 = |\psi_-(0)|^2$  for some arbitrary value of  $x = a$ . Another way of stating this is

$$\psi_+(a) = e^{i\tilde{k}a}\psi_-(0) \quad (8)$$

for arbitrary  $\tilde{k}$  and  $a$ . Plugging into the wave function (6) then yields

$$\cos \tilde{k}a - \cos ka = \frac{V_0}{k} \sin ka, \quad (9)$$

which gives  $\tilde{k}$  and  $a$  as implicit function of  $k$ . For a chain of such potentials, it should be clear that the wave function will be periodic everywhere (and the state therefore of extended character) only if all the  $a_i$ 's and all the  $V_i$ 's are equal. Otherwise (i.e. for *any* disorder, all wavefunctions obeying the usual boundary conditions must fall off exponentially at large distances, i.e. they represent localized states. *Any* statistical distribution of  $a_i$ 's and/or  $V_i$ 's lead to localization in 1D.

### 6.2.1 Anderson model

Anderson (1958)<sup>3</sup> investigated a model which contains some features of the disorder in real 3D systems, and in the process proposed the first quantitative definition of localization. Instead of moving some of the ionic positions away from the regular lattice, he considered a *periodic* lattice and a Hamiltonian  $H$  consisting of an ordinary periodic kinetic energy  $-t \sum_i c_i^\dagger c_{i+1} + h.c.$  but random site energies  $V_i$ .<sup>4</sup> Only for the special case that all  $V_i$  are equal can we say with certainty that energy bands are formed and all states are extended (Bloch waves). But what happens (Anderson asked) if we now assume the  $V_i$  are statistically distributed according to

$$P[V_i] = \begin{cases} \frac{1}{W} & |V_i| \leq \frac{W}{2} \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

Anderson now proposed calculating the probability  $P$  that a particle, beginning at  $t = 0$  on site  $i$ , returns to the same site in the limit of long times  $t \rightarrow \infty$ . If this probability is nonzero ( $P > 0$ ), the particle is said to be localized, whereas if it is zero the particle is clearly in an extended state, where the chances of it returning is essentially zero.<sup>5</sup> I won't repeat the calculation but give the result and try to motivate it a bit. The answer is expressed in terms of the site energy variance  $W$  which appears in the probability distribution for

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<sup>3</sup>P.W.Anderson, Phys. Rev. 109, 1492 (1958)

<sup>4</sup>It is generally believed that, since translational invariance is destroyed, models of this type are equivalent to more physical models as depicted e.g. in Figure 1

<sup>5</sup>This definition therefore clearly has the virtue of describing in a simple way why it is much more likely in low dimensions, particularly 1D, to find localized states.

the site energies. It is a measure of the average on-site energy fluctuation in the system, and, hence, the “amount of disorder”. A second energy is the bandwidth  $D$  of the unperturbed kinetic energy (for a 3D n.n. tight binding model it would be  $D = 8t$ —check!). Anderson’s calculation yielded a sharp *localization transition*: for  $W/D \lesssim 5$  extended states existed, while for  $W/D \gtrsim 5$  they disappeared. In other words, there is a sharp boundary in energy between localized and extended states. If an eigenstate lies below the threshold energy (“mobility edge”),  $E \lesssim E_c \simeq W/5$ , it is localized, whereas if its energy  $E > E_c$ , it is extended (see figure 3). How can

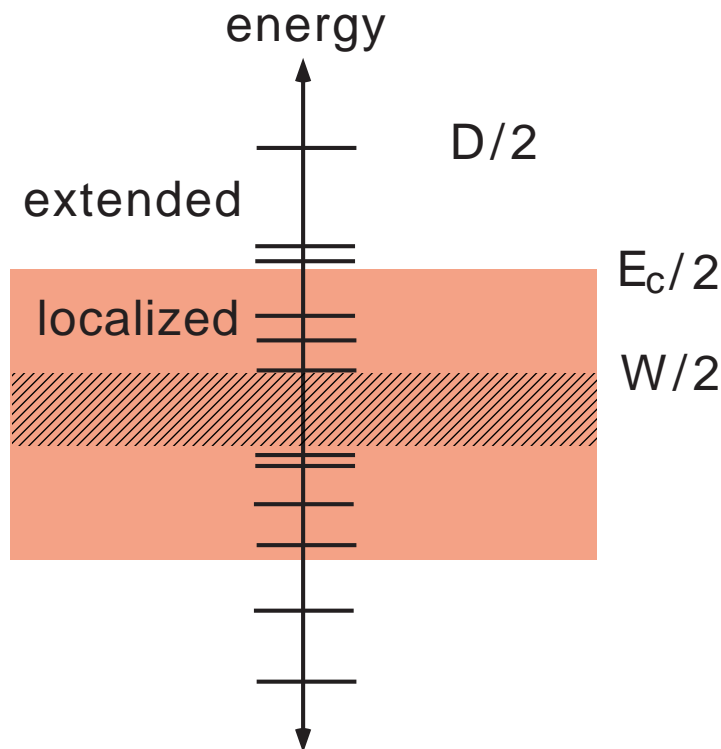


Figure 3: Random energy levels of Anderson model with disorder  $W$  and bandwidth  $D$ .

this transition be induced in practice? Either by increasing the disorder level, or by tuning the characteristic energy of

electrons ( $E_F$ ) through the mobility edge.

What we actually measure to exhibit the transition is of course the conductivity. The DC conductivity of a  $D$ -dimensional system is

$$\sigma_0 = \frac{e^2}{h} \frac{a^{2-D}}{\pi} \frac{\ell}{a} \equiv \sigma_c \frac{\ell}{a}, \quad (11)$$

where  $\ell = v_F \tau$ ,  $v_F = \hbar k_F / m$ , and  $k_F = \pi / a$ . Note the quantity  $\sigma_c$  is *universal* in the sense that it doesn't depend on disorder through  $\ell$ . The disorder dependence comes in only through the ratio  $\ell/a$ . But recall that the original derivation of the Drude conductivity was via the Boltzmann equation, where we had to assume  $\ell/a \gg 1$  (Ioffe-Regel criterion). Mott therefore postulated that there would be a minimum possible metallic conductivity  $\sigma_{min} \lesssim \sigma_c$ . Mott argued that as one approached the transition from the metallic side, the conductivity would decrease proportional to  $\ell$  and then when  $\sigma = \sigma_{min}$ , would drop discontinuously to zero (1st order transition), as shown in Figure 4. Experiments in recent years have shown that it is at least possible to obtain conductivities well below the minimum value suggested by Mott, and generally supported Anderson's picture of a continuous transition. In Figure 4 b) are shown data where the metal-insulator transition was tuned in Si by addition of donor P atoms and the conductivity of different samples thus prepared compared with Mott's prediction. ?? Question— Resistivity saturation?



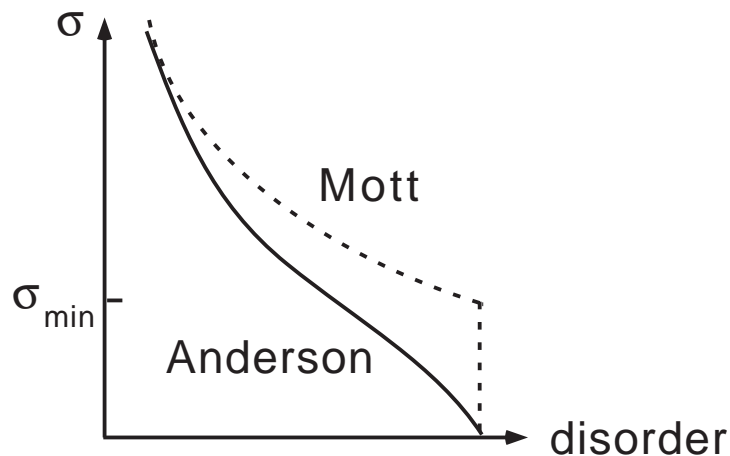


Figure 4: a) Approach of the conductivity to the localization transition; b) Experiments of Rosenbaum (1980) and Palanen (1982) on Si:P.

### 6.2.2 Weak Localization

Let us now consider the localization problem a bit more carefully, starting from the metallic side far from the transition where it is more tractable. Our goal will be to understand the so-called *quantum corrections* to the Drude conductivity  $\sigma_0$ , i.e. corrections of relative order  $1/(k_F\ell)$  or higher in the regime where such an expansion is applicable. We start from what is sometimes called the Edwards, or binary alloy model, where a few pointlike scatterers of equal strength  $V_0$  are randomly distributed over a periodic lattice. We want to know the conductivity  $\sigma$  or diffusion coefficient  $D$  for such a system, recalling that the two properties should be related by the Einstein relation

$$\sigma = e^2 N_0 D \quad (12)$$

where  $N_0$  is the density of states at the Fermi level as usual.

In this case let's take a dimensionless measure of disorder  $\lambda \sim n_i V_0^2 / E_F^2$ , where  $n_i$  is the impurity concentration. This parameter is sometimes called the “coupling constant” or “disorder strength” in this type of model. For  $D = 1$  we saw that arbitrarily weak disorder strength  $\lambda \rightarrow 0$  leads to localization. The “critical value” of disorder  $\lambda_c$  above which one finds localization, is zero. In  $D = 3$  we know  $\lambda_c$  is different from zero, since for sufficiently weak  $\lambda$  we know we find metallic behavior, i.e. nonzero  $\sigma$  at  $T \rightarrow 0$ . What about  $D = 2$ , which appears to be a marginal case? This is a difficult question, which is still at the center of many debates (although the problem without interactions appears to have been resolved). Is there an Anderson transition in  $D = 2$ ? Is  $\lambda_c = 0$  or  $> 0$ ?

Let's start with very weak disorder  $\lambda \ll 1$ . We *assume* metallic behavior, and that effects of disorder can be treated perturbatively far from any Anderson transition. This will be true in 3D; we don't know if it works in 2D or not yet. Weak disorder can also be expressed in terms of the mean free path being much longer than the interparticle distance, i.e.  $k_F \ell \gg 1$ , or equivalently  $E_F \tau \gg 1$ . For concreteness, let's choose  $\lambda = (2\pi E_F \tau)^{-1}$ , and try to calculate the “precursor” effects of localization, i.e. the corrections  $\delta\sigma$  to the conductivity

$$\sigma = \sigma_0 + \delta\sigma, \quad |\delta\sigma| \ll \sigma_0. \quad (13)$$

These corrections are commonly referred to as “weak localization effects”. We'd like to know how  $\delta\sigma$  depends not only on disorder, but also other external parameters we can control, like system size  $L$ , frequency  $\omega$ , temperature  $T$ , and magnetic

field  $H$ .

### **Diffusion of quantum particles**

The Drude conductivity from which we begin is proportional to the inverse coupling constant as mentioned before,

$$\sigma = \frac{e^2}{h} \frac{a^{2-D}}{\pi} \frac{\ell}{a} \propto \frac{1}{\lambda} \quad (14)$$

Recall in the Boltzmann approach which led to this result consecutive collisions of particles are taken to be uncorrelated, i.e. multiple scattering is not taken into account. If there is a finite probability for such processes to occur, this result should be corrected. To see what we are missing, we examine the diffusion of a particle in a  $D$ -dimensional disordered system. Suppose that at time  $t = 0$  the particle is located at  $\mathbf{r}_0$ . The particle diffuses away at later times, and we assume that its position can only be described statistically by a smooth probability distribution  $P(\mathbf{r}, t)$  which obeys the diffusion equation:

$$\frac{\partial P}{\partial t} - D_0 \nabla^2 P = 0, \quad (15)$$

where the diffusion constant is given by  $D_0 = v_F^2 \tau / d$ ,  $v_F$  is the characteristic velocity of the particles (in this case the Fermi velocity). The explicit solution of (15) is

$$P(\mathbf{r}, t) = \frac{e^{-\frac{|\mathbf{r} - \mathbf{r}_0|^2}{4D_0 t}}}{(4\pi D_0 t)^{D/2}} \quad (16)$$

For long times the exponential is unimportant, so that

$$P(\mathbf{r}, t) \propto \frac{1}{V_{diff}} = \begin{cases} (D_0 t)^{-1/2} & D = 1 \\ (D_0 t)^{-1} & D = 2 \\ (D_0 t)^{-3/2} & D = 3 \end{cases} \quad (17)$$

Note  $V_{diff}$  is the  $D$ -dimensional diffusion volume in which the particle has diffused after a long time  $t$ .<sup>6</sup> So far everything we have said is purely classical. To understand what might change for a quantum particle, consider how different paths between different points contribute to the total probability (see figure 5). The trajectories have a typical uncertainty which is of course zero in the classical case, but something like a Fermi wavelength  $\lambda_F = \hbar/(mv_F)$  in the quantum case. Thus we can think of these paths as being really tubes of probability flux with finite diameter. Furthermore, we will assume that along each tube the quantum mechanical *phase* is preserved, i.e. we are at low enough temperatures such that the inelastic scattering rate is much larger than the elastic one,  $\tau_{in} \gg \tau$ . There is for each path or “tube” a probability amplitude, and the total transport probability from A to B is just

$$W = |\sum_i A_i|^2 = \sum_i |A_i|^2 + \sum_{i \neq j} A_i A_j^*. \quad (19)$$

The first term represents noninterfering trajectories, i.e. the classical case when the tubes are infinitely narrow. The second term describes the quantum-mechanical interference pro-

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<sup>6</sup>Note probability is normalized  $\int d^D r P = 1$  at any time, so at long times when  $P$  no longer depends on  $r$ , we essentially have

$$\int_{V_{diff}} P = V_{Diff} P = 1 \quad (18)$$

cesses, neglected in the analysis of the Boltzmann equation. Usually this analysis is fully justified, since each path carries a different phase, and when one adds up all the paths the phases cancel, i.e. the interference is totally destructive.

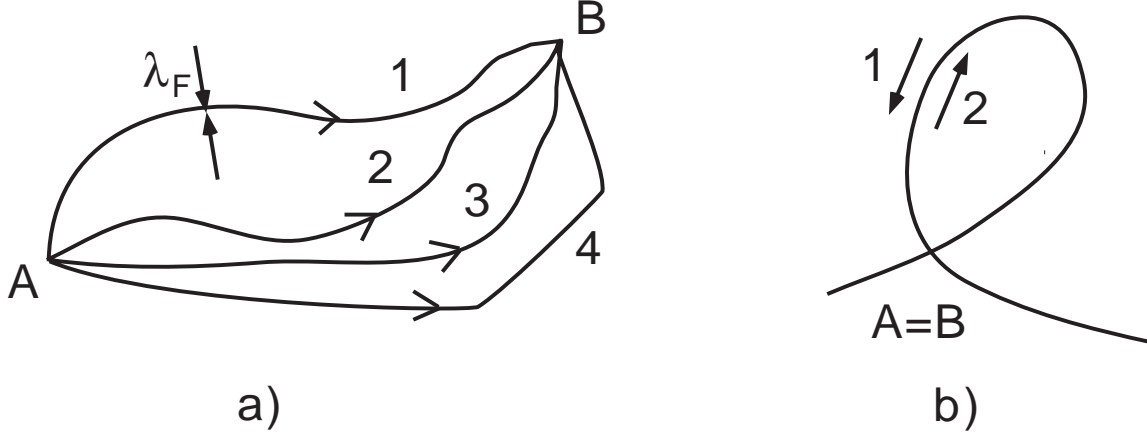


Figure 5: a) Diffusion paths between A and B; b) time-reversed return paths.

In one special case one can see this is not true. Suppose points A and B are the same, i.e. we are interested in the return probability as discussed above. Time reversal invariance now tells us that the paths 1 and 2 shown have identical amplitudes  $A_1 = A_2 = A$ , including in particular identical phases, leading to *constructive* interference for the two processes. The probability of return is therefore  $2|A|^2$  in the classical case and  $2|A|^2 + 2A_1A_2^* = 4|A|^2$  in the quantum case. Therefore

$$W_{QM} = 2W_{classical} \quad (20)$$

Thus it appears that quantum-mechanical diffusion must be slower than classical diffusion due to these multiple scattering processes alone; one can think of the effect we just described as an additional backscattering effect which does not exist in the

classical case. There is a correspondingly *lower* conductivity in the quantum case.

One should remark that the above result obtains simply because we allowed different trajectories between any two points to interfere. This is a quantum effect in the case of electrons because we have accounted for their wave nature. However in the case of wavelike phenomena of any type, including those thought of as classical in nature, like the propagation of light, the same effects will occur. It is possible to observe “localization” of classical light waves by looking for coherent backscattering in a disordered medium, say scattering of light by tiny polystyrene spheres in aqueous suspension. The transmission is reduced from the amount predicted by an incoherent scattering calculation by just the right amount due to constructive interference of light waves travelling on closed, time-reversed paths just as in the case of weak localization of electrons.

**Conductivity correction.** We now need to be a bit more quantitative and try to estimate the size of the corrections to  $\sigma_0$  due to these effects. Due to the above discussion we expect the sign of the correction  $\delta\sigma$  to be negative. To do this we need to estimate the probability of the closed configurations among all configurations contributing to  $\sigma$ . First note that the interference contribution of two tubes is proportional to their intersection volume. But the return path tubes are unique in that their entire volume is necessarily an intersection with a time-reversed path. What we’ll do is simply calculate

the ratio of the volume of a small element of the return tube to the entire diffusion volume the particle could occupy at a time  $t$  (which includes all paths). This is the probability that a particle will return & intersect itself during the diffusion. As shown in Figure 6, the volume of the tube  $dV$  swept out

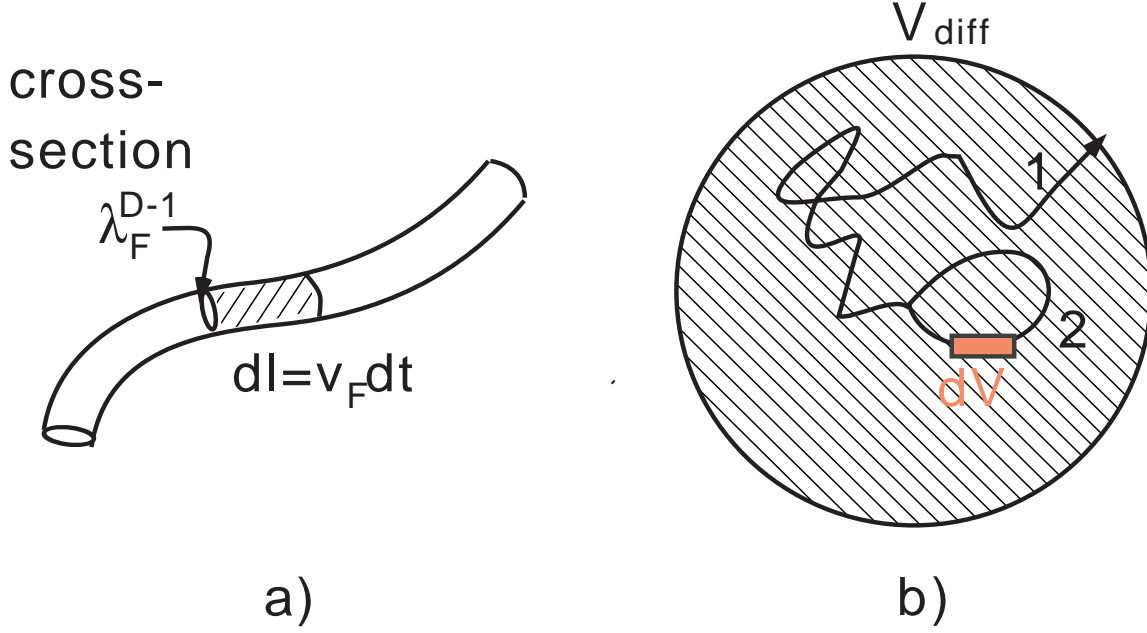


Figure 6: a) small volume element of return path tube; b) comparison of total diffusion volume with that of return path tube.

by the particle in a time  $dt$  is the cross section  $\lambda_F^{D-1}$  times the length swept out  $v_F dt$ , so the probability is

$$P_{closed} = \int_{\tau}^{\tau_{in}} \frac{dV}{V_{diff}} = v_F \lambda_F^{D-1} \int_{\tau}^{\tau_{in}} \frac{dt}{(D_0 t)^{D/2}}, \quad (21)$$

where the lower limit  $\tau$  is essentially set by the time the particle starts diffusing, and the upper one by the time where phase-breaking scattering destroys the phase coherence of the individual trajectories and hence the possibility of interfer-

ence. Performing the integrals, we obtain

$$\frac{\delta\sigma}{\sigma_0} \propto -\lambda \times \begin{cases} \left(\frac{\tau_{in}}{\tau}\right)^{1/2} & D = 1 \\ \log\left(\frac{\tau_{in}}{\tau}\right) & D = 2 \\ \left(\frac{\tau_{in}}{\tau}\right)^{-1/2} & D = 3 \end{cases} \quad (22)$$

To get a feeling for what these mean and how big they might be, assume that the inelastic relaxation rate is some power of the temperature  $\tau_{in}^{-1} \sim T^p$  (for electron-phonon collisions it would be  $p = 3$  ( $T \ll T_D$ ), for electron-electron  $p = 2$ ). Then

$$\frac{\delta\sigma}{\sigma_0} \propto -\lambda \times \begin{cases} T^{-p/2} & D = 1 \\ \frac{p}{2} \log\left(\frac{\tau}{T}\right) & D = 2 \\ T^{p/2} & D = 3 \end{cases} \quad (23)$$

### Remarks:

- Corrections all *decrease* conductivity, consistent with expectation that quantum effects amount to additional source of backscattering relative to Drude (classical) result.
- In  $D = 3$  these corrections are negligible at low  $T$ .
- In this approximation the correction is linear in the disorder parameter  $\lambda$
- For  $D = 1$ , the correction is actually classical (since tubes have zero diameter); also the result is divergent, consistent with full localization in 1D.
- In 2D, correction is logarithmic but also leads to divergent result. We are therefore not allowed to use the weak localization result in 2D below a temperature set roughly



by  $\sigma_0 \simeq \delta\sigma$ . In particular, we are not allowed to draw conclusions about whether all states are localized or not at  $T = 0$ .

- We needed to assume time reversal invariance to make the argument above, which is not correct in the presence of magnetic field (see below).

### 6.2.3 Scaling theory of localization

An answer to the question of what happens in 2D, as well as many other questions, was provided by the scaling theory of localization<sup>7</sup> The approaches to the problems discussed above are mostly suited either to the metallic or the insulating side of the metal-insulator transition, but are not capable of discussing what happens at the transition itself. Abrahams et al. (the so-called “gang of four”) drew upon ideas about phase transitions which had been developed in the late 60’s and 70’s by Fisher, Kadanoff and others, which proposed that because phase transitions involved fluctuations on all length scales, properties of the system would become scale-invariant. Scaling theories asked how properties of the system changed as the size of the system was increased, and made *scaling hypotheses* regarding the functional independence of these properties of microscopic system parameters near the transition.

Abrahams et al. chose as an appropriate property the *conductance*  $g = 1/R$  of a hypercube of side  $L$  ( $R$  is the resistance), whose importance for the localization problem had

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<sup>7</sup>Abrahams, Anderson, Licciardello & Ramakrishnan (1979).

been pointed out by Thouless. We know two limits of how  $g$  depends on system size. In the metallic (ohmic) regime,  $g \sim L^{D-2}$ ,<sup>8</sup> whereas in the localized regime because the wavefunctions have a characteristic size  $\xi$  the conductance must scale exponentially  $g \sim \exp(-L/\xi)$  for  $L \gg \xi$ . How can we interpolate between these two known cases? Assume we have a hypercube of side  $L$  and conductance  $g(L)$ , and ask how the conductance  $g(bL)$  of a larger hypercube of side  $bL$  ( $b > 1$  is a scale factor) depends on the conductance of the starting cube. In principle,  $g(bL)$  *could* depend not only on the *value* of the conductance  $g(L)$  at the smaller scale, and the length  $L$  itself, but on lots of other microscopic properties,  $g(bL) = f[g(L), L, \tau, k_F, \dots]$ . But let's assume that near the transition the behavior is universal, i.e. the only relevant parameter is the  $g$  of the smaller system, i.e.

$$g(bL) = f(b, g(L)), \quad (24)$$

or equivalently

$$g(L) = f[b, g(L/b)], \quad (25)$$

and  $f$  is some function. Eq. 25 is what we mean by the scaling hypothesis of Abrahams et al., from which the entire theory follows. Note that the relation should hold for any  $b$ , so that there is nothing to prevent us from differentiating both sides with respect to  $b$ , and then setting  $b=1$ . Then we obtain

$$\frac{dg(L)}{d \log L} = f_1[g(L)] \quad (26)$$

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<sup>8</sup>Recall from freshman physics that for a resistor  $R = \rho L/A$ , where  $L$  is the length and  $A$  is the cross-sectional area. For a cube  $R = 1/g \sim L^{-1}$ , so  $g \sim L$ .

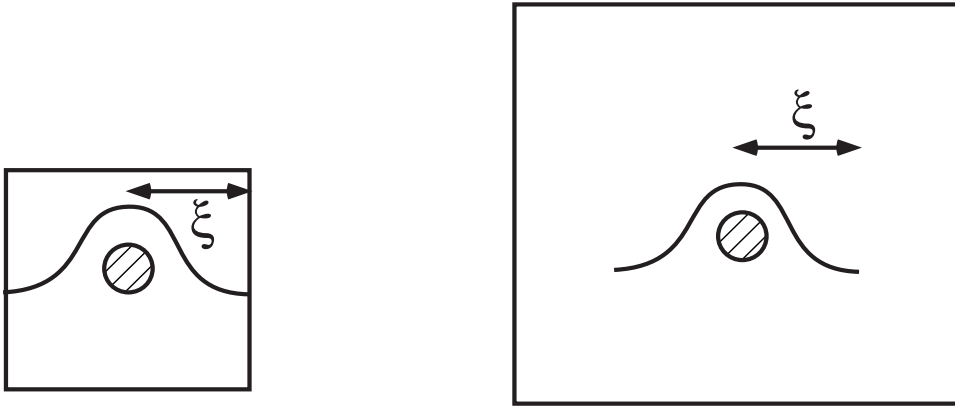


Figure 7: Schematic localized wavefunction in two different size systems.

where  $f_1$  is a new function of  $g$  involving  $f$ . Thus the logarithmic derivative of  $g$  depends only on  $g$  itself, and not on any other length scales! Abrahams et al. defined a  $\beta$  function (the name comes from renormalization theory):

$$\beta = \frac{1}{g} \frac{dg(L)}{d \log L} = \frac{d \log g(L)}{d \log L} = f_2[g(L)], \quad (27)$$

where  $f_2$  is a new function which is still only dependent on  $g(L)$ . The  $\beta$  function has known limits based on what we have already figured out about  $g$ :

$$\beta = \begin{cases} \log g & \text{localized} \\ D - 2 - \frac{c(D)}{g} + \mathcal{O}\left(\frac{1}{g^2}\right) & \text{metallic,} \end{cases} \quad (28)$$

where  $c(D)$  is a dimension-dependent factor which controls the weak-localization corrections discussed in the previous section. Already at this stage it is reasonable to guess a smooth interpolation between these limits. The guess of Abrahams et al. is sketched in Figure 8.

What do these curves mean? Note if  $\beta > 0$ , it means that

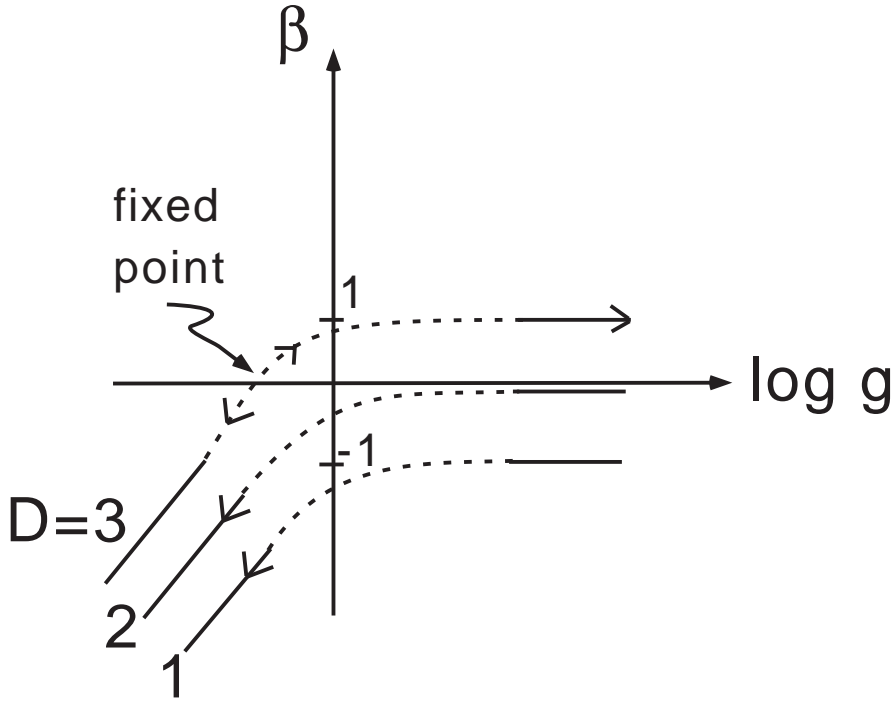


Figure 8:  $\beta$ -function prediction of scaling theory of localization. Solid lines correspond to analytic estimates made in text.

$dg/d\log L > 0$  since  $g > 0$  always. This means that increasing the system size increases the conductance. Look for example at the  $D = 3$  case above the point where the curve crosses the  $\beta = 0$  axis. Any  $\log g$  corresponds to a particular  $L$  since the curve is monotonic; increasing the system size from here *increases the conductivity*, hence moving you to the right along the curve. This is the meaning of the arrows pointing to the right on this curve above  $\beta = 0$ . The system “flows” towards metallic behavior as you go towards the thermodynamic limit. Every other point on all the curves shown corresponds to  $\beta < 0$ , so the arrows point the other way: as you increase the system size, the conductivity *decreases*, i.e the system “flows” towards localized behavior. Only the  $D = 3$  curve has a “fixed point (unstable)” with  $\beta = 0$  where

the flow moves away in both directions. This point indicates the existence of an Anderson transition in 3D.<sup>9</sup>

What about 2D? Can we induce a transition between metallic and localized behavior in very thin films? The foregoing considerations suggest the answer is no. Note the  $\beta$  – *function* for 2D is always negative, i.e. the system always becomes localized as you increase the size. It is interesting to connect this discussion to the preceding one on weak localization. We knew from classical considerations in the strongly metallic regime only that  $\beta \rightarrow 0$  as  $\log L \rightarrow \infty$ . The sign of the weak localization correction to the  $\beta$ -function,  $-c(2)/g$ , with  $c(2) > 0$ , indicates that even if, at a given system size  $L$ , the conductance were huge, the “flow” would be towards localized behavior, i.e. for macroscopic film sizes there should be no extended states.<sup>10</sup> Thus the weak localization calculation is extremely important even though we said it only strictly applies in the “perturbative regime”.<sup>11</sup>

Returning to 3D for a moment, we note that information about the transition itself can be extracted. Near the fixed

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<sup>9</sup>The terms “flow” and “unstable fixed point” come from the theory of Wilson’s renormalization group (RG), where the meaning is only slightly different. Usually when studying RG flows, we are looking at the transformation of a set of parameters describing how the system’s Hamiltonian changes as the scale is changed, or, what is frequently equivalent, energy or temperature is reduced. See e.g. N. Goldenfeld, *Lectures on the Renormalization Group*

<sup>10</sup>At this writing the existence of metallic behavior in 2D is still controversial. In 199x, experiments by Kravtsov?, Sarachik, and Pudalov? suggested that a transition to metallic behavior was possible even for very thin films. Some theorists believe this is a genuine metal-insulator transition in 2D which violates the predictions of the scaling theory because the effects of electron-electron interactions, not accounted for in the scaling theory, are important enough to slightly shift the marginal behavior of the  $\beta$ -function so that a fixed point is created. Others believe the experiments can be explained by traps or other “ $T$ -dependent disorder, a picture which implies that the apparent metallic behavior must disappear at sufficiently low temperatures.

<sup>11</sup>We said before the weak localization calculation started in the “metallic regime”. In 2D this means in the regime where  $g$  is large, even though the system is never truly metallic.

point, the  $\beta$ -function can be linearized as

$$\beta = \frac{1}{\nu} \left( \frac{g - g_c}{g_c} \right), \quad (29)$$

where  $1/\nu$  is defined to be the slope at the transition,  $d\beta/d\log g|_{\log g_c}$ . We can integrate this to find

$$\frac{L}{L_0} = \left( \frac{g - g_c}{g_0 - g_c} \right)^\nu, \quad (30)$$

where  $g_0 = g(L_0)$ . In the localized regime, we substitute the assumed form  $g$

#### 6.2.4 Universal conductance fluctuations

#### 6.2.5 Effect of Magnetic Field

#### 6.2.6 $hc/e$ and $hc/2e$ oscillations

### 6.3 Quantum Hall effect

## 6.4 Mesoscopic transport

#### 6.4.1 Coulomb blockade

# 1 2nd quantization and stat mech (continued)

## 1.1 Appendix. Free Fermi Gas

The hamiltonian is

$$H_0 = \sum_{\mathbf{k}\sigma} \tilde{\epsilon}_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (1)$$

where

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu. \quad (2)$$

The mean value will be

$$\langle H_0 \rangle = \sum_{\mathbf{k}\sigma} \tilde{\epsilon}_{\mathbf{k}} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle = \sum_{\mathbf{k}\sigma} \tilde{\epsilon}_{\mathbf{k}} n_{\mathbf{k}\sigma}^0 \quad (3)$$

where

$$n_{\mathbf{k}\sigma}^0 = \frac{1}{e^{\tilde{\epsilon}_{\mathbf{k}}/T} + 1} \quad (4)$$

At  $T \rightarrow 0$  and in 3D

$$\sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} = \frac{3}{5} \epsilon_F. \quad (5)$$

Derive  $\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = n_{\mathbf{k}}^0$  (neglect spin).

## 1.2 Appendix. Free Bose Gas

“Same” Hamiltonian

$$H_0 = \sum_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \quad (6)$$

where  $a_{\mathbf{k}}$  has bosonic commutation relations. Here we have

$$n_{\mathbf{k}}^0 = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = \frac{1}{e^{\beta \tilde{\epsilon}_{\mathbf{k}}} - 1}. \quad (7)$$

The density of states for a 3D gas is

$$N(\epsilon) \equiv \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) = \frac{1}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} \quad (8)$$

so by applying the conversion

$$\sum_{\mathbf{k}} \rightarrow \int \frac{d^3k}{8\pi^3} = \int d\epsilon N(\epsilon) \quad (9)$$

we have

$$\langle n \rangle = c \int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\beta(\epsilon - \mu)} - 1} \equiv n \quad (10)$$

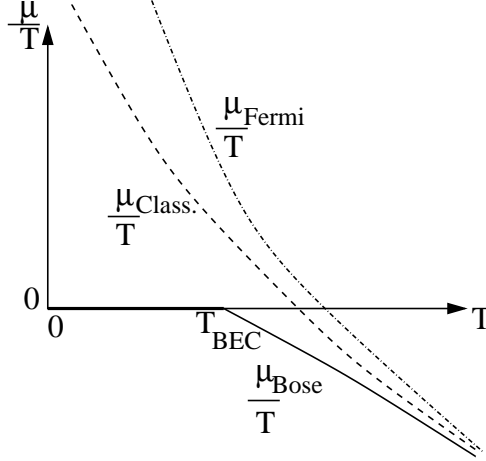


Figure 1: Chemical potentials of free homogeneous Bose, classical, and Fermi gases  $\mu_i/T$  vs. temperature  $T$ .

and we can solve for  $\mu$ . Note due to the negative sign in the denominator  $\mu$  must always be negative otherwise the occupation number  $n_{\mathbf{k}} < 0$  for some  $\mathbf{k}$ . Note further there is a problem as  $T \rightarrow 0$ , with  $\epsilon > \mu$ , instead of being equal to zero we have  $\langle n \rangle \rightarrow 0$  rather than a fixed number. That means there is no solution for  $\mu$ . Where is the error? We forgot the possibility of macroscopic occupation of the ground state, i.e.

$$\sum_{\mathbf{k}} n_{\mathbf{k}} \rightarrow n_0 + c \int_{0+}^{\infty} d\epsilon \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)} - 1}. \quad (11)$$

We can extract the critical temperature that this can happen by taking the limit  $n_0 \rightarrow 0$  which will determine the onset of the Bose-Einstein condensation (BEC) temperature while  $\mu = 0$ . In other words

$$n = cT_0^{3/2} \underbrace{\int_0^{\infty} dx \frac{x^{1/2}}{e^x - 1}}_{\zeta(3/2)\Gamma(3/2)} \quad (12)$$

which means that for the 3D parabolic band case we have  $T_0 \sim n^{2/3}$ .

## 2 Confinement of atoms and BEC

### 2.1 History of BEC

1908 Discovery of superfluid  $^4\text{He}$  (“He-II”).

1938 F. London suggests He-II = BEC but in liquid state that means there are strong interactions present and  $n_0(T=0) \ll 1$ .



1959 Hecht: spin-polarized H might remain gaseous to low T: 2 H $\uparrow$  atoms can not form H<sub>2</sub>.

1980 Silvera and Walraven stabilize H $\uparrow$ .

80's Search for methods to confine H $\uparrow$   $\rightarrow$  magnetic traps (Kleppner Graytak).

1989 Dehmelt and Paul Nobel prize for ion traps.

1995 BEC in laser traps: C. Wiemann, E. A. Cornell(Rb), W. Ketterle(Na).

2001 Nobel prize to Wiemann, Cornell, Ketterle

## 2.2 Atom confinement

In modern laser or magnetic traps atoms are confined in an approximately harmonic potential. Let us compare the DOS for harmonic trap and free gas in a box with hard walls.

Free gas (3D)	Harmonic trap
$H = \sum_i \frac{\mathbf{p}_i^2}{2m}$	$H = \sum_i \left\{ \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}m(\omega_1^2 x_i^2 + \omega_2^2 y_i^2 + \omega_3^2 z_i^2) \right\}$
	$\epsilon_{n_1, n_2, n_3} = \hbar\omega_1(n_1 + \frac{1}{2}) + \hbar\omega_2(n_2 + \frac{1}{2}) + \hbar\omega_3(n_3 + \frac{1}{2})$
$N(\epsilon) = \frac{m^{3/2}}{\sqrt{2\pi^2}}\epsilon^{1/2}$	$N(\epsilon) = \frac{1}{2\omega_1\omega_2\omega_3}\epsilon^2$

Aside from the power law  $N(\epsilon) \sim \epsilon^{\alpha-1}$  in DOS, there should be little qualitative difference in 2 noninteracting systems, so let us redo the BEC for a general  $N(\epsilon) = C_\alpha \epsilon^{\alpha-1}$ .

$$N = N_{ex}(T_c, \mu = 0) = \int_0^\infty d\epsilon N(\epsilon) \frac{1}{e^{\epsilon/T_c} - 1} = C_\alpha T_c^\alpha \underbrace{\int_0^\infty dx \frac{x^{\alpha-1}}{e^x - 1}}_{\Gamma(\alpha)\zeta(\alpha)} \quad (13)$$

so we have

$$T_c \sim N^{1/\alpha}. \quad (14)$$

In other words for the free gas  $T_c \sim N^{2/3}$  while for the harmonic trap  $T_c \sim N^{1/3}$ .

For a 2D free gas  $N(\epsilon) \sim \text{const.}$  and

$$\int_0^\infty dx \frac{1}{e^x - 1} = \infty \quad (15)$$

so there is no BEC in a 2D free gas except at  $T=0$ . But in a 2D harmonic trap  $N(\epsilon) \sim \epsilon$  so  $\alpha = 2$  and  $T_c \sim N^{1/2}$ . This does not violate theorems we will encounter later about lack of long range order in 2D at finite  $T$  because the system is not infinite in extent.

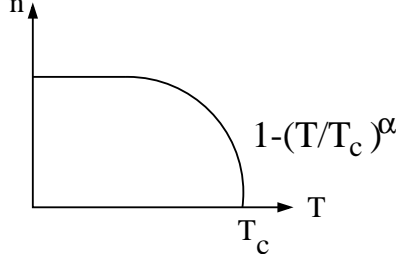


Figure 2: Condensate fraction vs.  $T$  for gas with  $N(\epsilon) \sim \epsilon^{\alpha-1}$  density of states.

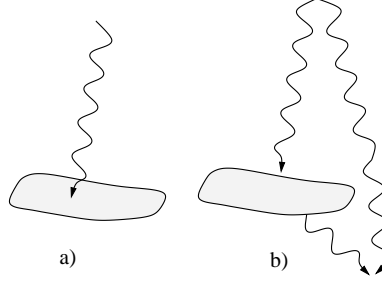


Figure 3: Two different methods of detecting condensate in atomic clouds with laser: a) direct measurement of absorption profile, suffers from heating effects; b) phase contrast imaging.

## 2.3 Condensate fraction

For  $T < T_c$  so that  $\mu = 0$  the number of excited particles will be

$$N_{ex}(T) = C_\alpha \int_0^\infty d\epsilon \epsilon^{\alpha-1} \frac{1}{e^{\epsilon/T} - 1} \quad (16)$$

which converges for  $\alpha > 1$  into the value

$$N_{ex} = C_\alpha \Gamma(\alpha) \zeta(\alpha) T^\alpha \quad (17)$$

so we get

$$N_0 = N - N_{ex} = N \left[ 1 - \left( \frac{T}{T_c} \right)^\alpha \right]. \quad (18)$$

## 2.4 Density profile and velocity distribution

Or, how to tell if you have a BEC!

The density profile of the trapped cloud is measured with a laser.

### 2.4.1 Ground state profiles

Lowest SHO eigenfunction is

$$\phi_0(\mathbf{r}) = \frac{1}{\pi^{3/4}(a_1 a_2 a_3)^{1/2}} e^{-\frac{x^2}{2a_1^2}} e^{-\frac{y^2}{2a_2^2}} e^{-\frac{z^2}{2a_3^2}} \quad (19)$$

where

$$a_i = \sqrt{\frac{1}{m\omega_i}} \sim 10^{-1} \mu m. \quad (20)$$

The density profile is  $n_0(\mathbf{r}) = |\phi_0(\mathbf{r})|^2$  or in momentum space

$$n_0(\mathbf{p}) = N |\phi_0(\mathbf{p})|^2 = \frac{N}{\pi^{3/4} c_1 c_2 c_3} e^{-\frac{p_x^2}{c_1^2}} e^{-\frac{p_y^2}{c_2^2}} e^{-\frac{p_z^2}{c_3^2}} \quad (21)$$

where

$$c_i = \frac{1}{a_i}. \quad (22)$$

This is a Maxwellian distribution with effective “temperatures”  $T_i = \omega_i/2$ . The main point is that the velocity and density distributions are in general anisotropic ( $x, y, z$  are different).

### 2.4.2 Semiclassical ( $T \gg T_c$ ) profiles

In this case we have

$$n(r) = \frac{1}{Z} \int d^3 p e^{-\beta H} \sim e^{-V(r)/T} = e^{-\frac{x^2}{R_1^2}} e^{-\frac{y^2}{R_2^2}} e^{-\frac{z^2}{R_3^2}} \quad (23)$$

where

$$R_i^2 = \frac{2T}{m\omega_i^2}. \quad (24)$$

but the momentum distribution will be

$$n(p) = \frac{1}{Z} \int d^3 r e^{-\beta H} \sim e^{-p^2/2mT} \quad (25)$$

that means isotropic.

**Remarks.** The size of the cloud of the thermal excitations is  $\gg$  the size of the condensate. Quantum mechanically we have SHO levels, where the size of the  $n$ th level is  $\langle r \rangle_n \sim \sqrt{n} a_0$  with  $a_0 = \sqrt{1/m\omega_0}$  for the isotropic case. The thermal occupation of the levels gives  $n\omega_0 \sim T$  so we have

$$\langle r \rangle_n \sim \sqrt{\frac{T}{\omega_0}} a_0 \sim R_i \text{ (from semiclassics)} \quad (26)$$

so the semiclassical approximation is justified for excitations as long as  $T/\omega_0 \gg 1$ , which is well satisfied for most traps. Typical values are  $T \sim \mu K$  and  $\omega_0 \sim 10^3 \text{ Hz} \simeq nK$ . To detect BEC we create a cloud, and allow it to expand. The condensate will be highly anisotropic, but since  $n(p)$  for the thermal excitations is isotropic, the cloud of excitations becomes isotropic.

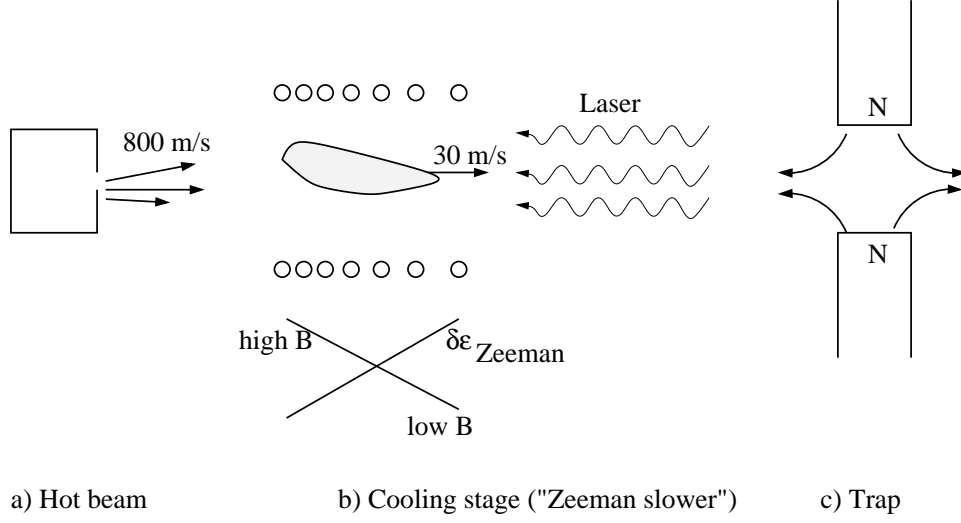


Figure 4: Basic configuration for creating, cooling and trapping alkali gases (schematic) note in particular I have left out possible evaporative cooling stage, and depicted only a simple quadrupole trap.

## 2.5 Trapping and cooling of atoms

Evaporate atoms from the surface of alkali metal ( $\sim 600\text{K}$ ). Usually the two-body recombination times are slow (of the order of the age of the universe!) because it is hard to satisfy conservation laws. The three-body recombination times are of the order of minutes, so experiments must be done during this time. The system is in principle not stable but metastable.

For the cooling the atoms absorb light and slow down. For the absorption we need  $\omega = E_{n+1} - E_n$ . The velocity dispersion in the cloud causes a Doppler broadening  $\delta\epsilon_D$  where

$$\delta\epsilon_D = -\mathbf{k} \cdot \mathbf{v} \quad (27)$$

while  $\mathbf{v}$  is the atom velocity and  $\mathbf{k}$  the laser wave vector. For the absorption in the lab frame we have

$$\gamma_p = \frac{\gamma/2}{1 + [2(\omega - \omega_0 + \delta\epsilon_D)/\gamma]^2} \quad (28)$$

where  $\omega - \omega_0$  is referred as “detuning” and  $\omega_0$  is the rest frame resonant frequency. For maximum deceleration we have  $\omega - \omega_0 + \delta\epsilon_D \leq \gamma$  and makes the laser resonant with atoms in their rest frame and we will have

$$\mathbf{F} = \hbar\mathbf{k}\gamma_p \Rightarrow \mathbf{F}_{max} \rightarrow \frac{\hbar\mathbf{k}\gamma}{2} \quad (29)$$

As atoms in the beam slow down, the changing  $\delta\epsilon_D$  takes them out of resonance so they can not cool further. To compensate for that we can introduce an inhomogeneous magnetic

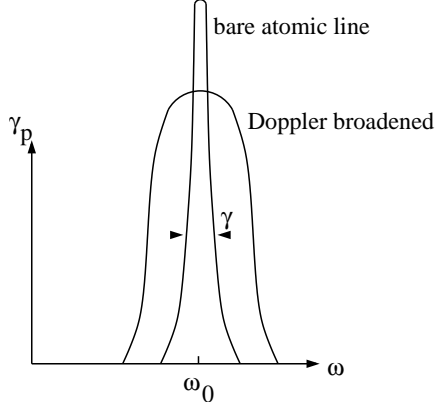


Figure 5: Spectrum of atomic transition with and without Doppler broadening.

Figure 6: a) Quadrupole trap; b) Ioffe-Pritchard trap.

field—“Zeeman cooler”. As the atom slows down, it progresses further along the path and the Doppler  $\delta\epsilon_D$  decreases but  $\delta\epsilon_{Zeeman} = -\mu \cdot \mathbf{B}$ . We choose  $B$  and  $B'$  to keep the cloud together on resonance. The result is a cooling down to 30 m/s.

### 2.5.1 Magnetic traps

The design is a combination of wires and coils to trap some atoms through the Zeeman interaction. So spin-up atoms are attracted to regions of low field while spin-down are repelled. No static field configuration with maximum, can find minimum. The simplest quadrupole trap is

$$\mathbf{B} = B'(x, y, -2z) \rightarrow B = B'(x^2 + y^2 + 4z^2)^{1/2}. \quad (30)$$

We have assumed that  $\mu$  aligns itself with the local field and follows the field lines so  $\delta\epsilon_{Zeeman} = |\mu||B|$ ,  $\mu < 0$ . Then the spin-up state atoms seek the lowest field *magnitude*.

Problem:  $t$ -dependent  $B$  field causes spin-up go to spin-down transitions. When  $\omega_{eff} \sim \delta\epsilon_{Zeeman}$  arises since particles are moving in inhomogeneous field. Trap losses in vicinity of minimum with  $B = 0$ .

Solution: “Plug hole”:

- TOP trap (time-averaged orbiting potential) use quadrupole but apply rotating homogeneous field to move position of node in  $t$  dependent way. If  $\omega \ll \mu\langle B \rangle$  the rotating field itself won’t cause transitions.

- Ioffe-Pritchard trap: First try two Helmholtz coils, same sense then

$$B = \text{const}_1 + 3\text{const}_2(z^2 - \frac{1}{2}\rho^2) \quad (31)$$

The result is that it doesn't trap in both directions  $z, \rho$ . Add four wires then

$$B = c_1 + 3c_2(z^3 - \frac{1}{2}\rho^2) + \frac{c^2}{\rho^2}. \quad (32)$$

Can now choose  $c$  such that trap is confining, i.e. that coeff. of  $\rho^2$  is positive, and it will have desired minimum at  $|B| > 0$ .

### 2.5.2 Optical traps:

Atom with energies  $E_0, E_1$  in presence of a laser field

$$H_{Dipole} = -\mathbf{p} \cdot \mathcal{E}(t) \quad (33)$$

The idea is that the electric field  $\mathcal{E}$  polarizes the atom

$$\alpha(\omega) = \frac{|\langle 1|\mathbf{p} \cdot \hat{\mathcal{E}}|0\rangle|^2}{E_1 - E_0 - \omega + i\gamma/2}, \quad (34)$$

where  $\gamma$  is the natural lifetime of the excited state in the absence of the laser field, and  $\omega$  is the laser frequency. Shift  $\Delta E_0$  by

$$\Delta E_0 = -\frac{1}{2}\alpha'(\omega)\langle \mathcal{E}(t) \rangle_t = \frac{\Omega_R^2 \delta}{\delta^2 + \gamma^2/4} \quad (35)$$

and the transition rate of atoms leaving the ground state is

$$\gamma_g = \frac{1}{\hbar}\alpha''(\omega)\langle \mathcal{E}^2 \rangle \quad (36)$$

while the ‘‘Rabi’’ frequency is  $\Omega_R = \langle 1|\mathbf{p} \cdot \mathcal{E}_\omega|0\rangle$  and the detuning  $\delta = \omega - \omega_0$  while  $\omega_0 = E_1 - E_0$ . So  $\Delta E_0$  is less than zero if  $\delta < 0$ – ‘‘red detuning’’. Spatial variation of  $E_0$  leads to trapping, i.e.  $-\nabla E_0$  gives a restoring force near center of laser beam.

A focussed laser field produces an electric field profile with maximum at one point; for red detuning atoms are attracted to the center. Detuning is also necessary to prevent absorption pressure and heating. To give concrete numbers, take example of Na, trap has laser wavelength  $\lambda \sim 985$  nm while laser wavelength  $\lambda_0 \sim 589$  nm (Na d-line). The depth of the optical trap is determined by  $\delta E_0$  at the center, of order  $\mu K$  in this case.

## 2.6 Scattering theory

The particle wave function after the scattering event will be of the form

$$\psi = e^{ikz} + f(\theta) \frac{ikr}{r} \quad (37)$$

For low energies we will have s-wave scattering only which means that  $f(\theta)$  will become a constant of order  $a$ , the s-wave scattering length. The wave function will become

$$\psi \rightarrow 1 - \frac{a}{r}, \quad (38)$$

where the last term is the asymptotic outgoing scattered wave  $\psi_{sc}$ . If we define  $\chi = r\psi$  then  $\chi \sim r - a$  and  $a$  will become the  $r$ -intercept of the radial function  $\chi$ . The general wave function has the form

$$\psi = \sum_{lm} R_l \psi_{lm} \quad (39)$$

where

$$R_l \sim e^{i\delta_l} \frac{\sin(kr - l\pi/2 + \delta_l)}{kr} \quad (40)$$

and for  $l = 0$  we will have

$$\begin{aligned} \chi &= re^{i\delta_0} \frac{\sin(kr + \delta_0)}{kr} = re^{i\delta_0} \frac{\sin kr \cos \delta_0 + \sin \delta_0 \cos kr}{kr} \xrightarrow{k \rightarrow 0} re^{i\delta_0} \left[ \cos \delta_0 + \frac{\sin \delta_0}{kr} \right] \\ &= re^{i\delta_0} \cos \delta_0 \left[ 1 + \frac{\tan \delta_0}{kr} \right] \equiv re^{i\delta_0} \cos \delta_0 \left[ 1 - \frac{a}{r} \right] \end{aligned} \quad (41)$$

so the definition of  $a$  is

$$a = -\frac{\tan \delta_0}{k} \quad (42)$$

and for weak scattering we have  $\delta_0 \sim -ka$ . For the scattering energy we have

$$\epsilon_k^0 = \frac{k^2}{2\mu} = \frac{k^2}{m} \quad (43)$$

where  $\mu = m/2$  is the reduced mass. If we go back to Schrödinger's equation now we have

$$(\epsilon_k^0 - \epsilon_{k'}^0) \psi_{sc}(k') = U(k'k) + \sum_{k''} U(k'k'') \psi_{sc}(k'') \quad (44)$$

and Fourier transforming it using

$$\psi_{sc}(k) = \int d^3r e^{-ikr} \psi_{sc}(r) \quad (45)$$

we will get the formal solution

$$\psi_{sc}(k') = (\epsilon_k^0 - \epsilon_{k'}^0 + i\delta)^{-1} T(k', k, E = \epsilon_k^0) \quad (46)$$

where the “T-matrix”  $T(k, k'; E)$  satisfies (matrix eqn. in k-space!)

$$T = U + U \sum_{k''} \frac{1}{E - \epsilon_{k''} + i\delta} T \quad (47)$$

For weak scattering ( $k \rightarrow 0$ ) we can use the Born approximation  $T(k, k') = U(0, 0)$  and get

$$\begin{aligned} \psi_{sc}(r) &= \sum_{k'} e^{ik'r} \psi_{sc}(k') = - \sum_{k'} e^{ik'r} \frac{U(k', 0)}{\epsilon_{k'}^0} \simeq -mU(0, 0) \underbrace{\sum_{k'} \frac{e^{ik'r}}{k'^2}}_{1/4\pi r} \\ &= -\frac{mU(0, 0)}{4\pi r} \equiv -\frac{a}{r} \end{aligned} \quad (48)$$

in other words

$$a = \frac{mU(0, 0)}{4\pi}. \quad (49)$$

For a more general calculation we can replace  $U$  by an effective potential.

## 2.7 Effective potential and scattering length

Problem The bare interaction between two atoms is well known at large distances and possibly known at short distances. (Van der Waals)

If we define the dimensionless strength parameter  $C_6$  and using Bohr’s radius  $a_0 = \hbar^2/m_e e^2$  we can form the quantity  $\alpha = C_6 e^2 a_0^2$  characterizing the Van der Waals energy strength. By dimensional analysis we can find the length scale of the interactions. Since the kinetic energy is  $\sim \frac{\hbar^2}{mr_0^2}$  while the potential energy is  $\sim \frac{-\alpha}{r_0^6}$  we have a minimum when

$$r_0 \sim \left( \frac{\alpha m}{\hbar^2} \right)^{1/2} = \left( \frac{C_6 m}{m_e} \right)^{1/4} a_0 \gg a_0. \quad (50)$$

So the length scale which is approximately  $r_0 \sim 10^2 a_0$ . Below is a table of the  $C_6$  values for various elements.

Element	$C_6$
H	6.5
Li	1393
NA	1556
K	3897
Rb	4691
Cs	6851

A few remarks are in order.

- 1) Clouds themselves are at least 10 times bigger.



- 2) The strength of the Van der Waals forces are  $\sim \frac{1}{(\Delta E_{res})^3}$ . Hydrogen has smaller  $C_6$  because the 1s-2p transition is lowest, not ns $\rightarrow$ np!

Question: How can we calculate energy shifts due to interactions without knowing the details of the short range potential?

Answer: Introduce an “effective interaction” that describes the interactions between long wavelength degrees of freedom accounting for the short wavelength ones. Short distances are “integrated out”.

Our goal is to show that we can work with an effective potential of the form

$$\tilde{U}(r) = \frac{4\pi\hbar^2 a}{m} \delta(r) \quad (51)$$

where  $a$  is the s-wave scattering length which is defined in terms of the asymptotic large- $r$  part of the radial wavefunction  $\chi(r) = r\psi_{sc}(r)$  but depends sensitively on the short-distance behavior of the bare potential. If scattering is not weak a similar calculation gives  $\psi_{sc}(r) = -\frac{mT(0,0)}{4\pi r}$  which leads to

$$a = \frac{mT(0,0)}{4\pi}. \quad (52)$$

The low-energy  $T$ -matrix is the “effective potential” in the sense that it gives the exact result for  $\delta E$  when inserted for  $U$  in the Born approximation result for  $\psi_{sc}$  if the atoms are far apart. So if we are interested in the limit of interactions via long wavelength excitations we see that  $\tilde{U}$  (the effective potential in  $k$ -space) will be equal to

$$\tilde{U}_0 \equiv \frac{4\pi a}{m} = T(0,0). \quad (53)$$

The energy shift  $\delta E \sim \langle \Psi | \tilde{U}(r) | \Psi \rangle$  will then be (sum over all pairs of scatterers):

$$\delta E \sim \frac{1}{2} \frac{4\pi a}{m} \sum_{ij} |\Psi(r_{ij} \rightarrow 0)|^2. \quad (54)$$

To illustrate the dependence of  $a$  on short distances, we take a crude model of the Van der Waals potential

$$V(r) = \begin{cases} \infty & r < r_c \\ -\frac{\alpha}{r^6} & r > r_c \end{cases} \quad (55)$$

which reproduces the correct large-distance behavior. The scattering equation for the radial wave function is

$$\chi''(r) + \left[ k^2 - \frac{l(l+1)}{r^2} - 2m_r U(r) \right] \chi(r) = 0, \quad (56)$$

where  $m_r$  is reduced mass, and for  $k = l = 0$  and  $r > r_c$  we will have

$$\chi''(r) + \frac{2m_r \alpha}{r^6} \chi(r) = 0. \quad (57)$$

So  $\chi$  at large distances will be of the form  $\chi = c_1 r + c_2$  and if we define  $r_0 = (2m_r \alpha)^{1/4}$  (check dimensions!) and  $x = r/r_0$  we end up with a relatively simple eqn.

$$\chi''(x) + \frac{1}{x^6} \chi(x) = 0. \quad (58)$$

The solution of the above differential equation with the boundary condition that  $\chi$  should go to zero at  $r_c$  is

$$\chi(x) = A x^{1/2} \left[ J_{1/4}\left(\frac{1}{2x^2}\right) - \frac{J_{1/4}\left(\frac{1}{2x_c^2}\right)}{J_{1/4}\left(\frac{1}{2x_c^2}\right)} J_{-1/4}\left(\frac{1}{2x^2}\right) \right] \quad (59)$$

where  $x_c = r_c/r_0$ . The asymptotic large- $r$  behavior is extracted using the Bessel-function asymptotic formula

$$J_p(z) \simeq \frac{z^p}{2^p \Gamma(1+p)} \quad (60)$$

and the result is

$$\chi \simeq A \frac{1}{\sqrt{2} \Gamma(5/4)} + B \frac{\sqrt{2}}{\Gamma(3/4)} \frac{r}{r_0}. \quad (61)$$

By definition we therefore get

$$a = r_0 \frac{\Gamma(3/4) \cos(r_0^2/2r_c^2 - \pi/8)}{2\Gamma(5/4) \cos(r_0^2/2r_c^2 - 3\pi/8)}. \quad (62)$$

The following remarks are in order:

- 1) The scale is set by  $r_0$
- 2)  $a$  depends on the details of the short-range part of  $U(r)$  via  $r_c$
- 3)  $a$  changes sign as  $r_c$  is varied
- 4) Divergence of  $a$  means a bound state.
- 5) The sign of  $a$  for fixed  $r_c$  depends on the energy of the highest bound state

## 2.8 Gross-Pitaevskii equation

The effective interaction at low energies is

$$U_0 = \frac{4\pi a}{m} \quad (63)$$

a constant in momentum space so a delta function in coordinate space

$$U(r - r') = U_0 \delta(r - r'). \quad (64)$$

We will follow the Hartree procedure and assume that the states are symmetrized products of single-particle wave functions. The ground state is a condensate which means that all bosons are in the same  $\phi_0(r)$  state. Notice that this takes care of the exchange symmetry the system should have. So the many body wave function will have the form

$$\Psi(r_1, \dots, r_N) = \prod_{i=1}^N \phi_0(r_i) \quad (65)$$

and the Hamiltonian

$$\sum_{i=1}^N \left[ \frac{p_i^2}{2m} + V(r_i) \right] + U_0 \sum_{i < j} \delta(r_i - r_j). \quad (66)$$

The ground state energy expectation value (Problem set) is

$$E \equiv \langle \Psi | H | \Psi \rangle = N \int d^3r \left[ \frac{1}{2m} |\phi_0|^2 + V(\mathbf{r}) |\phi_0|^2 + \frac{N-1}{2} U_0 |\phi_0|^4 \right]. \quad (67)$$

The error we make in this approximation is that we assumed  $N$  atoms in the condensate. In fact, interactions put some atoms in excited states, however it turns out that this is  $O(na^3)^{1/2} = O(a/r_s)^{3/2}$  which for  $a \ll r_s$  is very small. The typical Alkali scattering length is 30 – 100 Å. The densest gas obtained so far is  $n \sim 10^{15} \text{ cm}^{-3}$  which gives

$$r_s \sim 10^{-5} \text{ cm} = 10^3 \text{ Å}. \quad (68)$$

So the corrections are small, O(1-10%).

Since we have  $N$  atoms in the same quantum state it is tempting to define a single macroscopic wave function

$$\psi(r) = N_0^{1/2} \phi_0(r). \quad (69)$$

Do not confuse  $\psi(r)$  with the many-body wave function  $\Psi(r_1, \dots, r_N)$ . The normalization of  $\psi(r)$  is

$$\int d^3r |\psi(r)|^2 = N_0 = N \text{ (if } T=0 \text{ in Hartree approximation)} \quad (70)$$

so we have

$$n(r) = |\psi(r)|^2 \quad (71)$$

and  $\psi(r)$  is called the order parameter.

Formally this can be given precise meaning. From the one-particle density matrix

$$\begin{aligned} \rho(r, r') &\equiv N \int dr_2 \dots r_N \Psi^*(r, r_2, \dots, r_N) \Psi(r', r_2, \dots, r_N) \\ &\equiv \langle \hat{\Psi}^\dagger(r) \hat{\Psi}(r') \rangle \text{ (in 2nd quantized form)}. \end{aligned} \quad (72)$$

But  $\rho$  is hermitian so

$$\rho(r, r') = \sum_i n_i \chi_i^*(r) \chi_i(r') \quad (73)$$

so in BEC only one term of  $O(1)$  (except in the fragmented BEC case) will survive in the sum and

$$\rho(r, r') = N\chi_0^*(r)\chi_0(r') \equiv \psi^*(r)\psi(r'). \quad (74)$$

To produce the “Gross-Pitaevskii equations” we have to find the optimal  $\psi$  using the variation principle. This gives the result

$$\frac{\delta(E - \mu N)}{\delta\psi} = 0 \Rightarrow \quad (75)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi + U_0|\psi|^2\psi = \mu\psi. \quad (76)$$

We see that for a **uniform gas** case  $\nabla\psi = 0$  and  $V = 0$  and the solution becomes

$$\mu = U_0|\psi|^2 = nU_0. \quad (77)$$

For a **trap** the spatial extent of the cloud ( $\equiv R$ ) defines the scale of the kinetic energy  $\hbar^2/2mR^2$  and the potential energy  $m\omega_0^2 R^2/2$ . The typical size without the interactions is the harmonic oscillator length  $a_{osc} = (\hbar/m\omega_0)^{1/2}$ . So a repulsive  $U_0$  adds a  $+U_0\frac{N}{R^3}$  term and shifts the minimum to larger  $R$ . The kinetic energy term becomes less important as a result of that shift. For the strong-coupling case  $U, V \gg$  kinetic energy. When can  $U, V$  be comparable?

$$\frac{NU_0}{R^3} = \frac{1}{2}m\omega_0^2 R^2 \Rightarrow \quad (78)$$

$$R \sim \left(\frac{2NU_0}{m\omega_0^2}\right)^{1/5} \sim (8\pi)^{1/5}a_{osc}\left(\frac{Na}{a_{osc}}\right)^{1/5} \gg a_{osc}. \quad (79)$$

This approximation is called Thomas-Fermi approx. So most experiments are performed in the regime where the kinetic energy term can be neglected, which means the clouds must be sufficiently large. Let us solve the Gross-Pitaevskii equation neglecting the kinetic energy term

$$\left[V + U_0|\psi|^2\right]\psi = \mu\psi. \quad (80)$$

The spatial dependence is driven by  $V$  and the solution of course is

$$n(r) = |\psi|^2 = [\mu - V]/U_0. \quad (81)$$

The “boundary of the cloud” is given by  $V(r) = \mu$  in this approximation. Obviously it fails in some surface layer of thickness  $\delta$ . Since the energy  $(V + U_0|\psi|^2)$  involves the mean density ( $|\psi|^2$ ) this is called the Thomas-Fermi approximation for the Gross-Pitaevskii equation. For the harmonic trap the size is given by

$$R_i = \sqrt{\frac{2\mu}{m\omega_i^2}}. \quad (82)$$

What about if the condensate is suppressed locally for example by a hard wall? Then it “heals” over a “coherence length”  $\xi$ . So let us forget the external field and compare the kinetic energy term with  $U$  near the wall. We see that

$$\frac{\hbar^2}{2m\xi^2} \sim nU_0 \Rightarrow \quad (83)$$

$$\xi^2 = \frac{\hbar^2}{2mnU_0} = \frac{1}{\delta\pi na}. \quad (84)$$

For most systems we have  $a \ll \xi \ll R$ .

### 2.8.1 Vortices

The time-dependent Gross-Pitaevskii equation will allow for vortex solutions with quantized circulation. These vortex excitations in the condensate can be created in practice by a “laser paddle”, simply inserting a laser beam off-axis and “stirring”. The analogy with the Schrödinger equation is straight-forward and we can write

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi + U_0|\psi|^2\psi = i\hbar\frac{\partial\psi}{\partial t}. \quad (85)$$

If we multiply by  $\psi^*$  and subtract the complex-conjugate equation from it we end up with the current conservation equation

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0. \quad (86)$$

If we define  $\psi = fe^{i\phi}$  and since  $n = |\psi|^2$  we find

$$\mathbf{v} = \frac{\hbar}{m}\nabla\phi. \quad (87)$$

So  $\mathbf{v}$  is the gradient of a phase which means that  $\nabla \times \mathbf{v} = 0$  unless the phase  $\phi$  is singular. Notice that  $\nabla = \frac{1}{r}\frac{\partial}{\partial\phi}$  in cylindrically symmetric geometry.

Quantization of Circulation: The single valuedness of  $\psi$  requires

$$\oint_C \mathbf{v} \cdot d\mathbf{l} = \left\{ \frac{\hbar}{m} \int d\phi \frac{\partial}{\partial\phi} \phi \right\} = \frac{\hbar l}{m} \text{ (where } l \text{ is integer)} \quad (88)$$

$$\text{e.g., if } C = \text{circle} \quad (89)$$

Notice that we can define a “quantum of circulation” which is  $\frac{\hbar}{m}$  (by Feynman and Onsager). Notice as well that a simple azimuthal flow corresponds to

$$v2\pi r = \frac{\hbar l}{m} \Rightarrow \quad (90)$$

$$v = \frac{\hbar l}{2\pi m r}. \quad (91)$$

*N.B.* The kinetic energy diverges at  $r = 0$  so  $\psi$  must vanish there.

The total  $L = Nlh$  which corresponds to  $L/\text{particle} = lh$ . In general this is *not* true for asymmetrical flows but the overall circulation is still quantized.

The Gross–Pitaevskii equation in cylindrical coordinates for  $\psi = fe^{i\phi}$  is

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{\rho} \frac{d}{d\rho} \left( \rho \frac{df}{d\rho} \right) + \frac{d^2 f}{dz^2} \right] + \frac{\hbar^2}{2m\rho^2} l^2 f + Vf + U_0 f^3 = \mu f. \quad (92)$$

We examine 1st the  $l = 1$  vortex with no trap potential. If we would guess the length scale *a priori* it should be the coherence length  $\xi$  since  $\psi \rightarrow 0$  at the center. Let us scale all lengths with respect to  $\xi$ , and define  $x = \rho/\xi$  and also scale  $f$  by the known solution  $f_0 = \sqrt{\mu/U_0}$  for the rotation-free system, and put  $\chi = f/f_0$  (note this  $\chi$  is not the radial wave function!). The equation will transform to

$$-\frac{1}{x} \frac{d}{dx} \left( x \frac{d\chi}{dx} \right) + \frac{\chi}{x^2} + \chi^3 - \chi = 0. \quad (93)$$

At large distances we have

$$\chi^3 - \chi = 0 \Rightarrow \chi = 1. \quad (94)$$

At short distances we have

$$-x \frac{d}{dx} \left( x \frac{d\chi}{dx} \right) + \chi = 0 \Rightarrow \chi = x. \quad (95)$$

The energy density will be (in general, again—put back  $V$ , arb.  $\ell$ ).

$$\mathcal{E} = \frac{\hbar^2}{2m} \left[ \left( \frac{\partial f}{\partial \rho} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \right] + \frac{\hbar^2}{2m} l^2 \frac{f^2}{\rho^2} + Vf^2 + \frac{U_0}{2} f^4, \quad (96)$$

where  $f$  is now the solution to (95). If we set  $V = 0$  now, the energy/unit length of the  $l = 1$  vortex will be

$$\mathcal{E} = \int_0^b 2\pi\rho d\rho \left[ \frac{\hbar^2}{2m} \left( \frac{df}{d\rho} \right)^2 + \frac{\hbar^2}{2m} \frac{f^2}{\rho^2} + \frac{U_0}{2} f^4 \right], \quad (97)$$

where we have introduced the cutoff  $b$  to take care of the logarithmic divergence of the integrand ( $1/\rho^2$  term). Note the vanishing of the solution  $f$  at  $\rho \rightarrow 0$  regularizes the integral there. We are interested in the *extra* energy the vortex introduces into the system so we have to subtract off the “background”. Notice that this is not quite done by simply averaging the  $l^2/\rho^2$  term over all  $b$ , as you might think, since the asymptotic  $f$  is actually different (for fixed  $N$ ) since the vortex pushes the condensed particles out from the center. A careful subtraction gives

$$\epsilon_{\text{vortex}} = \pi n \frac{\hbar^2}{m} \log \left( 1.464 \frac{b}{\xi} \right). \quad (98)$$

Some remarks are in order.

- 1) The cutoff introduced for the divergence is the minimum of all the length scales of the system larger than  $\xi$  (system size, inter-vortex spacing).
- 2) If we redo the calculation for  $l \neq 1$  we find

$$\epsilon_{vortex} \simeq l^2 \pi n \frac{\hbar^2}{m} \log \left( \frac{b}{\xi} \right), \quad (99)$$

in other words it is always energetically favorable to put in many singly-quantized vortices.

#### Vortex in trap

The definition of  $\xi$  will be  $\frac{\hbar^2}{2m\xi^2} = \mu$  and by the Thomas–Fermi theory  $\mu = V(R) = \frac{1}{2}m\omega^2 R^2$ . So if we combine those two we will get

$$\frac{\xi}{R} = \frac{\hbar\omega}{2\mu}. \quad (100)$$

A similar calculation of the energy gives

$$\epsilon_v \simeq \pi n_0 \frac{\hbar^2}{m} \log \left( 0.888 \frac{R}{\xi} \right) \quad (101)$$

as expected the size of the cloud cuts off the divergence.

## 2.9 Remarks on conservation of angular momentum

The Hess–Fairbank experiment (see Leggett’s discussion) is the following. We start with a system of bosons rotating above  $T_c$  and wait for equilibrium to be established, assuming the annular container has thickness  $d \ll R$ . There is a critical angular velocity to stabilize the vortex with one quantum of circulation in this geometry. The energy of  $N$  particles of mass  $m$  (total mass  $M = Nm$ ) rotating with angular velocity  $\omega$  should be equal to the energy of  $N$  particles each with angular momentum  $\hbar$ :

$$\begin{aligned} N \frac{1}{2} m \omega^2 R^2 &= \frac{L^2}{2MR^2} = \frac{N\hbar^2}{2mR^2} \Rightarrow \\ \omega_c &= \frac{\hbar}{mR^2}. \end{aligned} \quad (102)$$

If the system rotates at  $\omega \ll \omega_c$  and we cool it down below  $T_c$ , the superfluid stops rotating in the lab frame because the angular momentum of it must be quantized and the closest quatum state is the  $l = 0$ .

Question: What happens to the “lost” angular momentum? In the  $^4\text{He}$  experiment it is transferred to the bucket, which actually speeds up! In BEC with no fixed container, the angular momentum can be taken up by elementary excitations of the condensate cloud of thermal nature ( $T > 0$ ), or by the center of mass motion. In the Hess–Fairbank case,

since  $\omega \ll \omega_c$ , the center of mass motion can not be excited since it carries  $L \sim N\hbar$ . Surface waves though, can carry away any number of  $\hbar$  quanta. In general, the state of the system is the combination of the above that minimizes the energy *i.e.* it can be calculated. (Analogy: the ground state in nuclear physics.)

Other alternatives:

- a) Evaporation.
- b) Circular polarization of optical trap photons.

In general the combination of these excitations which minimizes the ground state energy at fixed  $L$  is complicated (see “yrast” states in nuclear physics).

### 3 Interference of two condensates

Andrews *et al*, Science 275, 637 (1997)

Précis of experiment:

- 1) make trapped condensates by usual methods
- 2) separate with laser beam into two
- 3) release at  $t = 0$  and observe the overlapping condensates at time  $t$  with phase-contrast density measurements

If the two clouds may be thought of as two phase-coherent sources separated by  $\mathbf{d}$ , we can expect interference fringes

$$\psi = \sqrt{N_1}\varphi_1 + \sqrt{N_2}\varphi_2 \quad (103)$$

where  $\varphi_{1,2}$  are the single particle wave functions which we can assume initially to be Gaussians of size  $R_0$ . Then they spread as

$$\varphi_l = \frac{e^{i\phi_l}}{(\pi R_t^2)^{3/4}} e^{-\frac{[r+(-1)^l d/2]^2}{2R_t^2}} \left(1 + \frac{i\hbar t}{mR_0^2}\right) \quad (\text{where } l = 1, 2) \quad (104)$$

and

$$R_t^2 = R_0^2 + \left(\frac{\hbar t}{mR_0}\right)^2 \quad (\text{from elementary quantum mechanics}). \quad (105)$$

Density profile We have

$$n(r, t) = |\psi|^2 = N_1|\varphi_1|^2 + N_2|\varphi_2|^2 + 2\sqrt{N_1 N_2} \text{Re}[\varphi_1 \varphi_2^*]. \quad (106)$$

The interference term will be proportional to

$$\cos\left(\frac{\hbar}{m} \frac{\mathbf{r} \cdot \mathbf{d}}{R_0^2 R_t^2} t + \phi_1 - \phi_2\right) \quad (107)$$



the first fringe is when  $\frac{\hbar}{m} \frac{\Delta r d}{R_0^2 R_t^2} t = 2\pi$  which means

$$\Delta r = 2\pi \frac{m}{\hbar} \frac{R_0^2 R_t^2}{dt} \simeq \frac{\hbar t}{md} \text{ (for large } t) \quad (108)$$

which is observed by the experiment! But if clouds are well separated (tunneling time estimated to be  $>$  age of universe!), we should consider states with definite particle number  $N_1, N_2$  (more *a priori* realistic) we get a Fock state of the form

$$|N_1, N_2\rangle = \frac{1}{\sqrt{N_1! N_2!}} (a_1^\dagger)^{N_1} (a_2^\dagger)^{N_2} |0\rangle \quad (109)$$

where  $a_i^\dagger$  creates a particle in  $\varphi_i(\mathbf{r})$ . Again we can calculate the density by using the field operator

$$a_l^\dagger = \int d^3r \varphi_l(r) \hat{\psi}^\dagger(r) \quad (110)$$

and

$$\hat{\psi}(r)|N_1, N_2\rangle = \sqrt{N_1} \varphi_1(r) |N_1 - 1, N_2\rangle + \sqrt{N_2} \varphi_2(r) |N_1, N_2 - 1\rangle \quad (111)$$

and we will get

$$\begin{aligned} n(r) &= \langle N_1, N_2 | \hat{\psi}^\dagger(r) \hat{\psi}(r) | N_1, N_2 \rangle \\ &= N_1 |\varphi_1|^2 + N_2 |\varphi_2|^2 \text{ (no interference),} \end{aligned} \quad (112)$$

which means the sources are “totally incoherent”. What is going on?  $n(r)$  is the expectation value of the density operator *i.e.* the average over the result of many measurements. If we measure only once, as in the experiment we pick out one of the possible eigenvalues of the operator  $\hat{\psi}^\dagger(r) \hat{\psi}(r)$  with some probability.

In condensed matter we usually assume it is OK to replace averages over repetitions of the experiment by averages over all atoms. For example, if we measure the density of a crystal 20 times we will get the same result, with small  $O(1/N)$  quantum fluctuations, unobservable. This assumption can fail if the system is highly correlated, for example in a Bose condensate!

To detect interference in an experiment which averages over many runs, we should look at the operator which measures the fluctuations, namely

$$\begin{aligned} \langle N_1, N_2 | \hat{n}(r) \hat{n}(r') | N_1, N_2 \rangle &= (N_1 |\varphi_1|^2 + N_2 |\varphi_2|^2) (N_1 |\varphi'_1|^2 + N_2 |\varphi'_2|^2) - N_1 |\varphi_1|^2 |\varphi'_1|^2 \\ &\quad - N_2 |\varphi_2|^2 |\varphi'_2|^2 + \underbrace{2N_1 N_2 \text{Re}[\varphi_1^* \varphi_2 \varphi'_1 \varphi'_2]}_{\text{interference}}. \end{aligned} \quad (113)$$

Alternatively, in a “one-shot” measurement like Andrews et al. (only one cloud is split and the density profile measured after release), one should measure an interference pattern in a density measurement. Our claim is the following, if the experiments were repeated many times, we would get fringes each time, but with arbitrary relative phase, so the expectation value would then cancel such fringes.

# 1 Josephson Effect

In 1962 Brian Josephson<sup>1</sup>, then a 22-year old graduate student, made a remarkable prediction that two superconductors separated by a thin insulating barrier should give rise to a spontaneous (zero voltage) DC current,  $I_s = I_c \sin \Delta\phi$ , where  $\Delta\phi$  is the difference in phase across the junction. And that if a finite (DC) voltage were applied, an AC current with frequency  $\omega = 2eV/\hbar$  would flow.  $I_c$  is called the Josephson critical current.

There is a myth that Brian Josephson did his calculation (1962) and won the Nobel prize (1973) as part of the solution to a homework problem of Phil Anderson's. The truth is that Anderson was a lecturer on sabbatical at Cambridge in 1961-62, and he gave a series of lectures in which he mentioned the problem of tunneling between two superconductors, which Josephson then promptly solved. The idea was opposed at first by John Bardeen, who felt that pairing could not exist in the barrier region<sup>2</sup>. Thus much of the early debate centered on the nature of the tunneling process, whereas in fact today we know that the Josephson effect occurs in a variety of situations whenever two superconductors are separated by a "weak link", which can be an insulating region, normal metal, or short, narrow constriction.<sup>3</sup>

Let's first consider the last example as the conceptually simplest. The Ginzburg-Landau equation appropriate for this situation may be written

$$\xi^2 \frac{d^2 f}{dx^2} + f - f^3 = 0 \quad (1)$$

where  $\xi = \sqrt{\frac{\hbar}{2m^*a(T)}}$  is the GL coherence length and  $f(x) \equiv \Psi(x)/\Psi_\infty$ . Take  $L \ll \xi$ , so the deviations of  $\Psi$  coming from the bulk value  $\Psi_1$  of the first SC is small, and vice versa for the second SC. Changes of  $\Psi$  in the constriction occur over a length scale of  $L$ , so that the first term is of  $O((\xi/L)^2) \gg f - f^3$ . So we must solve a Laplace equation for  $f$ , ( $\frac{d^2 f}{dx^2} = 0$ )

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<sup>1</sup>Phys. Lett. 1, 251 (1962)

<sup>2</sup>Physics Today, July 2001

<sup>3</sup>In Je. 2009 I received an email from Brian Josephson correcting this version of the history:

Date: Wed, 10 Jun 2009 09:43:54 +0100  
From: Brian Josephson <bdj10@cam.ac.uk>  
To: pjh@phys.ufl.edu  
Subject: the Josephson myth  
Dear Peter,

While browsing I came across your mention of the 'myth' that I discovered the effect because of a problem set by Anderson. Your correction is not completely correct either! It was Pippard, my supervisor, who drew my attention to Giaever's tunnelling expts. and his theory, which started me thinking (especially as to how one could get away without using coherence factors). Anderson on the other hand told me of the Cohen/Falicov/Phillips calculation involving a single superconductor when it came out in PRL, which gave me the idea of how to do the two-sc. case. Previously I had got the broken symmetry idea which was crucial from a number of papers including Anderson's pseudospin model, and also expounded in his lecture course which I went to.

Best regards, Brian J.

with B.C.  $f(0) = 1$ ,  $f(L) = e^{i\Delta\Phi}$ . The solution will be

$$f = \left(1 - \frac{x}{L}\right) + \frac{x}{L}e^{i\Delta\phi}. \quad (2)$$

The solution can be thought of as two terms, the first  $\Psi_1$ , beginning to “leak” into the constriction from the left, the second  $\Psi_2$  leaking into the constriction from the right. The GL expression for the current will be

$$\begin{aligned} \mathbf{j} &= \frac{e^*\hbar}{2m^*i}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - \underbrace{\frac{e^{*2}}{m^*c}\Psi^*\Psi\mathbf{A}}_{\text{zero}} \\ &= \frac{e^*\hbar}{2m^*i}\Psi_\infty^2 \left[ \left(1 - \frac{x}{L} + \frac{x}{L}e^{-i\Delta\phi}\right) \left(-\frac{1}{L} + \frac{1}{L}e^{i\Delta\phi}\right) - c.c \right] \\ &= \frac{e^*\hbar\Psi_\infty^2}{m^*L} \sin \Delta\phi, \end{aligned} \quad (3)$$

which means that the current will be

$$I = I_c \sin \Delta\phi, \quad (4)$$

$$I_c = \frac{e^*\hbar\Psi_\infty^2}{m^*L}A, \quad (5)$$

where  $A$  is the cross-section.

Given that we have two weakly coupled QM systems, it is “not unreasonable” (justified by microscopic theory) to write down coupled Schrödinger equations

$$i\frac{\partial\Psi_1}{\partial t} = E_1\Psi_1 + \alpha\Psi_2 \quad (6)$$

$$i\frac{\partial\Psi_2}{\partial t} = E_2\Psi_2 + \alpha\Psi_1 \quad (7)$$

where  $H_0^{(i)}\Psi_i = E_i\Psi_i$  and  $E_1 = E_2 = E_0$  if the superconductors are identical. Take  $|\Psi_i|^2$  to be the density of pairs in  $\text{SC}_i$

$$\begin{aligned} \Psi_i &= \sqrt{n_i}e^{i\phi_i} \Rightarrow \dot{\Psi}_i = \frac{1}{2\sqrt{n_i}}\dot{n}_ie^{i\phi_i} + i\sqrt{n_i}\dot{\phi}_ie^{i\phi_i} \Rightarrow \\ \frac{\dot{n}_1}{2\sqrt{n_1}} + i\sqrt{n_1}\dot{\phi}_1 &= -iE_1\sqrt{n_1} - i\alpha\sqrt{n_2}e^{i(\phi_2-\phi_1)} \end{aligned} \quad (8)$$

$$\frac{\dot{n}_2}{2\sqrt{n_2}} + i\sqrt{n_2}\dot{\phi}_2 = -iE_2\sqrt{n_2} - i\alpha\sqrt{n_1}e^{i(\phi_1-\phi_2)}. \quad (9)$$

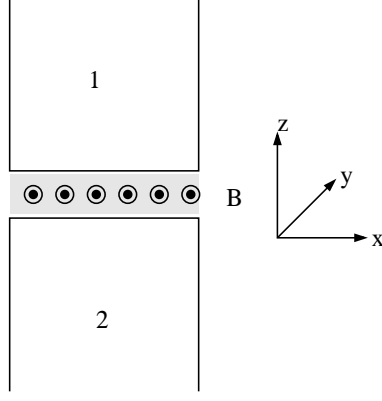


Figure 1:

If we take the real parts and use  $\dot{n}_1 = -\dot{n}_2$  we get

$$\begin{aligned} \frac{\dot{n}_1}{2\sqrt{n_1}} &= \alpha\sqrt{n_2} \sin(\phi_2 - \phi_1) \\ -\frac{\dot{n}_1}{2\sqrt{n_2}} &= \alpha\sqrt{n_1} \sin(\phi_1 - \phi_2) \Rightarrow \\ \dot{n}_1 &= 2\alpha\sqrt{n_1 n_2} \sin(\phi_2 - \phi_1), \end{aligned} \quad (10)$$

Note I've put  $V=A=1$ . Then the current is just  $j = 2e\dot{n}_1$ . If we take the imaginary parts we have

$$\sqrt{n_1}\dot{\phi}_1 = -E_1\sqrt{n_1} - \alpha\sqrt{n_2} \cos(\phi_2 - \phi_1) \quad (11)$$

$$\sqrt{n_2}\dot{\phi}_2 = -E_2\sqrt{n_2} - \alpha\sqrt{n_1} \cos(\phi_1 - \phi_2), \quad (12)$$

and by subtracting and assuming  $n_1 \simeq n_2$  (let's couple 2 identical superconductors at first) we get

$$\dot{\phi}_1 - \dot{\phi}_2 = E_2 - E_1 = 2e(V_1 - V_2) \quad (13)$$

where for the second equality we used the fact that the potential difference between the superconductors shifts the pair energies by  $-2eV$ . So we see that a finite voltage difference leads to a time changing phase difference  $\Delta\phi$  which means an AC current via Eq. (10).

Magnetic fields. Now put a flux through the junction where the  $\mathbf{B}$  field is along the  $-\hat{y}$  direction and  $A = -Bx\hat{z}$ . The phase of the wave function  $\Psi$  must change by

$$\phi \rightarrow \phi - \frac{2e}{c} \int d\mathbf{S} \cdot \mathbf{A} \quad (14)$$

for the theory to be gauge invariant. Notice that  $\phi$  is now space-dependent. So the Josephson

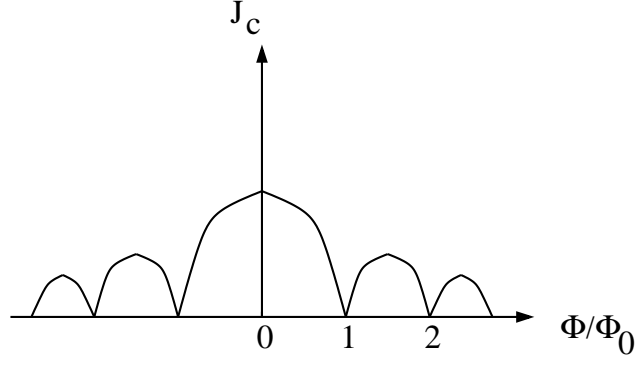


Figure 2:

equations will read

$$j = \underbrace{4e\alpha\sqrt{n_1n_2}}_{j_c} \sin \left( \Delta\phi - \frac{2e}{c} \int_1^2 d\mathbf{S} \cdot \mathbf{A} \right), \quad (15)$$

$$2e(V_1 - V_2) = \frac{\partial}{\partial t} \left( \phi_2 - \phi_1 - \frac{2e}{c} \int_1^2 d\mathbf{S} \cdot \mathbf{A} \right), \quad (16)$$

and since

$$\int_1^2 \mathbf{S} \cdot \mathbf{A} = \int_0^d dz (-Bx) = -Bxd, \quad (17)$$

we will have

$$\begin{aligned} J &= \int_0^L dx j(x) = \int_0^L dx j_c \sin \left( \Delta\Phi - \frac{2e}{c} Bxd \right) \\ &= \frac{Lj_c}{2\pi\Phi/\Phi_0} \left[ \cos \Delta\Phi - \cos \left( \Delta\Phi + \frac{2\pi\Phi}{\Phi_0} \right) \right], \end{aligned} \quad (18)$$

where  $\Phi_0 = \frac{2\pi c}{2e}$ . What is the maximum current through the junction for all possible  $\Delta\phi$ ?

We have to calculate  $\frac{dJ}{d\Delta\Phi} = 0$  which leads to the relation

$$\tan \Delta\Phi = \cot (\pi\Phi/\Phi_0) \quad (19)$$

and with a bit of tedious trigonometry to

$$J_c = Lj_c \left| \frac{\sin (\pi\Phi/\Phi_0)}{\pi\Phi/\Phi_0} \right|. \quad (20)$$

This formula produces the Josephson–Fraunhofer interference pattern. DC SQUID (Superconducting Quantum Interference Device)

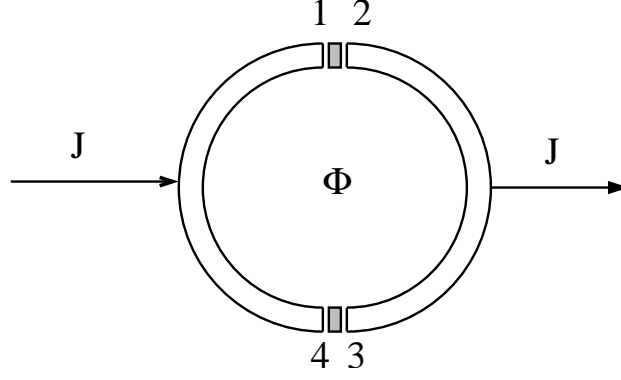


Figure 3:

We ignore resistance and capacitance for now. The inside SC thickness is assumed much greater than  $\lambda$  and since  $v_s = 0$  we have  $\nabla\phi = 2\mathbf{A}/\Phi_0$ . The flux will be

$$\begin{aligned}
 \Phi &= \oint d\mathbf{s} \cdot \mathbf{A} = \int_1^2 d\mathbf{s} \cdot \mathbf{A} + \frac{\Phi_0}{2} \int_2^3 d\mathbf{s} \cdot \nabla\phi + \int_3^4 d\mathbf{s} \cdot \mathbf{A} + \frac{\Phi_0}{2} \int_4^1 d\mathbf{s} \cdot \nabla\phi \\
 &= \frac{\Phi_0}{2}(\phi_3 - \phi_2) + \frac{\Phi_0}{2}(\phi_1 - \phi_4) + \int_1^2 d\mathbf{s} \cdot \mathbf{A} + \int_3^4 d\mathbf{s} \cdot \mathbf{A} \\
 &= \underbrace{\frac{\Phi_0}{2}(\phi_1 - \phi_2) + \int_1^2 d\mathbf{s} \cdot \mathbf{A}}_{\equiv -\gamma_{12}} + \underbrace{\frac{\Phi_0}{2}(\phi_3 - \phi_4) + \int_3^4 d\mathbf{s} \cdot \mathbf{A}}_{\equiv -\gamma_{34}} \\
 \Phi &= \gamma_{43} - \gamma_{12}.
 \end{aligned} \tag{21}$$

The Josephson current through the SQUID will be

$$\begin{aligned}
 J &= J_c (\sin \gamma_{12} + \sin \gamma_{43}) \\
 &= J_c (\sin \gamma_{12} + \sin(\gamma_{12} + \Phi)).
 \end{aligned} \tag{22}$$

Which means that the current oscillates with the flux. And as a result of that the SQUID can be a sensitive measure of magnetic fields. In practice we include the capacitance and resistance of the device.